

Chris G. Van de Walle

Materials Department, University of California, Santa Barbara, CA 93106-5050

Ph. (805) 893-7144; Fax (805) 893-8983

email: vandewalle@mrl.ucsb.edu

www.mrl.ucsb.edu/~vandewalle

EDUCATION

- 1986 Ph.D., Electrical Engineering, Stanford University, Stanford, California
1982 Burgerlijk Elektrotechnisch Ingenieur, Rijksuniversiteit Gent, Belgium

PROFESSIONAL EXPERIENCE

- 2015- Distinguished Professor, Materials Dept, University of California, Santa Barbara
2013- Herbert Kroemer Chair in Materials Science, Univ. of California, Santa Barbara
2004- Professor, Materials Department, University of California, Santa Barbara
1991-2004 Principal Scientist/Senior Member/Member of Research Staff, Xerox Palo Alto
Research Center, Palo Alto, California
1999 Alexander von Humboldt US Senior Scientist at the Fritz-Haber-Institut and the Paul-
Drude-Institut, Berlin, Germany, May-October 1999
1988-1991 Senior Member of Research Staff, Philips Laboratories, Briarcliff Manor, New
York; Joint-study agreement with IBM T. J. Watson Research Center
1991 Adjunct Professor, Columbia University, New York
1986-1988 Postdoctoral Scientist, IBM Research Division, T. J. Watson Research Center,
Yorktown Heights, New York
1983-1986 Consultant, Xerox Palo Alto Research Center, Palo Alto, California
1983-1986 Research Assistant, Stanford Electronics Laboratories, Stanford, California

HONORS

- National Academy of Engineering, 2016
- John Bardeen Award, TMS, 2015
- Medard W. Welch Award, AVS, 2013
- Fellow of the IEEE (2011), American Association for the Advancement of Science (2011),
Materials Research Society (2010), AVS (2009), American Physical Society (1997)
- PARC Excellence Award, 2003; PARC Golden Acorn Award, 2002
- David Adler Award, American Physical Society, 2002
- Humboldt Research Award for Senior US Scientist, Alexander von Humboldt Foundation,
Germany, 1998
- Graduate Student Award of the Materials Research Society, 1985
- F. E. Terman Award, Stanford University, Stanford, California, 1983
- Fellow, Belgian American Educational Foundation, 1982-1983
- Prijs van de Stad Gent (Prize of the City of Gent), Gent, Belgium, 1982

• **Plenary and Keynote Lectures:**

- 4th International Workshop on UV Materials and Devices (IWUMD4, Russia), 2019
- 7th International Symposium on Growth of III-Nitrides (ISGN, Poland), 2018
- 3rd International Conference on the Physics of 2D Crystals (ICP2C, Malta), 2018
- 15th International Conference on Advanced Materials (IUMRS-ICAM, Japan), 2017
- 12th International Conference on Nitride Semiconductors (ICNS, Strasbourg), 2017
- 59th Electronic Materials Conference (EMC, University of Notre Dame), 2017
- 10th International Conference on Computational Physics (ICCP10, Macao), 2017
- 26th Annual Meeting of MRS-J (Japan), 2016
- E-MRS Fall Meeting, Joint Session of Symposia C, M, and Z (Poland), 2016
- International Conference on Defects in Semiconductors (ICDS-28, Finland), 2015
- 9th International Conference on Computational Physics (ICCP9, Singapore), 2015
- International Conference on Nitride Semiconductors (ICNS-10, Washington, DC), 2013
- 7th Conf. of the Asian Consortium on Comput. Mater. Sci. (ACCMS-7, Thailand), 2013
- Europhysical Conf. on Defects in Insulating Materials (EURODIM, Hungary), 2010
- International Workshop on Nitride Semiconductors (IWN, Tampa, Florida), 2010
- International Conference on Defects in Semiconductors (ICDS-23, Japan), 2005
- 2nd International Symposium on Hydrogen in Matter (Uppsala, Sweden), 2005
- International Conference on SiC and Related Materials (ICSCRM, France), 2003
- International Conference on Physics of Semiconductors (ICPS-25, Japan), 2000
- International Conference on Defects in Semiconductors (ICDS-19, Portugal), 1997
- 1st Int'l Symp. on Ultra Clean Processing of Silicon Surfaces (UCPSS, Belgium), 1992

PROFESSIONAL ACTIVITIES

Conference chair:

- Co-Chair, ICMR Workshop on 'Ab-initio description of charged systems and solid/liquid interfaces for semiconductors and electrochemistry', Santa Barbara, July 7-11, 2014
- Co-Chair, CECAM Workshop on 'Which electronic structure method for the study of defects?', EPFL, Lausanne, June 8-10, 2009
- International Symposium on Materials Issues in Hydrogen Production and Storage, 2006
- Program Chair, 27th International Conference on the Physics of Semiconductors (ICPS), 2004
- Gordon Research Conference on Defects in Semiconductors, 1998
- 23rd Conference on Physics and Chemistry of Semiconductor Interfaces (PCSI), 1996
- 7th Trieste Semiconductor Symposium: Wide-Band-Gap Semiconductors, 1992

Organizer of Focused Sessions for the APS Division of Materials Physics, 1992, 1994, 1997

Proceedings Editor: 20th International Conference on Defects in Semiconductors, 1999; 27th International Conference on the Physics of Semiconductors, 2004; Workshop on 'Which electronic structure method for the study of defects?', 2009.

Member:

- APS (American Physical Society) – Fellow
- MRS (Materials Research Society) – Fellow
- AAAS (American Association for the Advancement of Science) – Fellow
- IEEE (Institute of Electrical and Electronics Engineers) – Fellow
- AVS – The Science and Technology Society – Fellow

PROFESSIONAL ACTIVITIES (CONT'D)

Program and Advisory Committees:

- International Conference on Defects in Semiconductors, 1995, 1999-2021
- International Workshop on UV Materials and Devices, 2019, 2020, 2022
- Materials Research Meeting, Yokohama, Japan, 2019
- Compound Semiconductor Week, Nara, Japan, 2019
- International Workshop on Gallium Oxide and Related Materials, 2017, 2019
- IUPAP Conference on Computational Physics, 2018, 2022
- Lawrence Symposium on Epitaxy, Scottsdale, Arizona, 2016, 2018
- SPIE Photonics West, Oxide-based Materials and Devices, 2018-2022
- Int'l Conf. on Superlattices, Nanostructures and Nanodevices, 2014, 2016, 2018, 2020, 2022
- International Symposium on Growth of III-Nitrides, 2008, 2015.
- International Ceramics Congress/Forum on New Materials, 2014, 2018, 2020, 2022
- Gordon Conf. on Defects in Semiconductors, 2008, 2010, 2012, 2014, 2016, 2018, 2020
- International Conference on Physics of Semiconductors, 2008, 2014, 2016
- Int'l. Workshop on Nitride Semiconductors, 2002, 2008, 2012, 2014, 2016, 2020, 2022
- International Conference on the Formation of Semiconductor Interfaces, 2009
- International Conference on II-VI Compounds, 1993, 1995, 2003
- International Workshop on Zinc Oxide, 2002, 2004, 2006
- International Symposium on Blue Laser and Light Emitting Diodes, 2000, 2002
- International Conference on Nitride Semiconductors, 2001, 2005, 2011, 2015, 2017, 2021
- International Workshop on Computational Electronics, 2001
- Conference on Semiconducting and Insulating Materials, 1998
- Electronic Materials Conference, 1995-1998
- International Conference on Computational Physics, 1997
- Conference on Physics and Chemistry of Semiconductor Interfaces, 1992-1996

Editorial and Advisory Boards, Committees:

- Vice-Chair (2015-2016), Chair-Elect (2016-2017), Chair (2017-2018), Past-Chair (2018-2019), APS Division of Computational Physics
- Associate Editor, Journal of Electronic Materials, 2011-2014
- IUPAP C8 Commission on Semiconductors, Vice-chair, 2005-2008; Member, 2008-2011
- US National Liaison Committee, National Research Council, 2005-2011
- Scientific Advisory Board, Paul Drude Institute, Berlin, Germany, 2002-2009
- Solid State Sciences Committee, Board on Physics and Astronomy, National Academies, 2003-2006
- Executive Committee, APS Division of Materials Physics, 2002-2004
- Editorial Board, Physical Review Letters, 1996-1999

Contracts and grants: National Science Foundation, Department of Energy, Department of Education, Office of Naval Research, Army Research Office, Air Force Office of Scientific Research, Intelligence Advanced Research Projects Activity, American Chemical Society, Semiconductor Research Corporation, University of California Energy Institute, Defense Advanced Research Projects Agency

PROFESSIONAL ACTIVITIES (CONT'D)

Referee/Reviewer:

- **Journals:** Annalen der Physik, Appl. Phys. A, Appl. Physics Lett., Appl. Surf. Sci., ChemPhysChem, Chem. Phys. Lett., Chem. Mater., Comput. Materials Sci., Computer Phys. Commun., ElectroChem. and Solid State Lett., EuroPhys. Lett., IEEE J. Quantum Electron., IEEE Trans. Electron Devices, Int'l J. Hydrogen Energy, Jap. J. Appl. Phys., J. Am. Ceram. Soc., J. Am. Chem. Soc., J. Appl. Phys., J. Chem. Phys., J. Chem. Theory and Comp., J. Crystal Growth, J. ElectroChem. Society, J. Electron. Mater., J. Luminescence, J. Mater. Res., J. Phys. Chem., J. Phys. Chem. Solids, J. Phys.: Condensed Matter, J. Phys. D: Appl. Phys., J. Vacuum Sci. Technol., Mater. Chem. Phys., Microelectron. Reliability J., Modeling and Simulation in Mater. Sci. Eng., Nano Lett., Nanotechnology, Nature, Nat. Mater., New J. Phys., Optics Commun., Physica B, Phys. Rev. B, Phys. Rev. Lett., Phys. Scripta, Phys. Status Solidi, Semicond. Sci. Technol., Solid State Commun., Solid State Ionics, Surf. Sci.
- **Funding agencies:** National Science Foundation, Department of Energy, Army Research Office, Office of Naval Research, Civilian Research and Development Foundation, International Science Foundation, Italian National Institute for Mater. Phys., Petroleum Research Fund, Research Corporation, Research Grants Council (Hong Kong), Science and Engineering Research Council (Singapore), Research Foundation Flanders, Swiss National Science Foundation, Science Foundation Ireland

RESEARCH INTERESTS

- Novel electronic materials; wide-band-gap semiconductors; oxides; two-dimensional materials; spin centers for quantum computing.
- Physics and chemistry of hydrogen interactions with solids, liquids, and molecular systems. Hydrogen generation and storage.
- Computational physics. Density-functional theory, pseudopotentials. Atomic and electronic structure of crystalline, polycrystalline and amorphous materials, interfaces, surfaces, defects.
- Semiconductor heterojunctions and superlattices; effects of strain; deformation potentials. Metal-semiconductor interfaces, Schottky barriers.
- Defects and impurities in solids, doping, diffusion. Hyperfine parameters, vibrational modes.
- Device simulations; optical gain in laser structures; loss mechanisms in light emitters.

PUBLICATIONS, PATENTS AND PRESENTATIONS

Over 500 scientific publications. 24 U.S. patents; several patents pending.

List of publications, patents, and invited talks at vandewalle.materials.ucsb.edu.

Over 230 Invited and Plenary Presentations at International Conferences and Schools.

Numerous invited seminars at universities and industrial or government laboratories.

Web of Science [March 2022]: *h* index: 107, Over 51,000 citations. 8 publications with over 1000 citations, 111 publications with over 100 citations.

Included in the 2014, 2017, 2018, 2019, 2020, and 2021 “[Highly Cited Researchers](#)” lists.

LIST OF PUBLICATIONS AND PRESENTATIONS

Chris G. Van de Walle

JOURNAL ARTICLES

1. “The significance of interference effects in thin film $\text{Cu}_2\text{S}/\text{CdS}$ solar cells”, C. Van de Walle and P. De Visschere, *Solar Cells* **9**, 353 (1983).
2. “Theoretical study of Si/Ge interfaces”, C. G. Van de Walle and R. M. Martin, *J. Vac. Sci. Technol. B* **3**, 1256 (1985).
3. “Theoretical calculations of heterojunction discontinuities in the Si/Ge system”, C. G. Van de Walle and R. M. Martin, *Phys. Rev. B* **34**, 5621 (1986). [doi: [10.1103/PhysRevB.34.5621](https://doi.org/10.1103/PhysRevB.34.5621)]
4. “Theoretical calculations of semiconductor heterojunction discontinuities”, C. G. Van de Walle and R. M. Martin, *J. Vac. Sci. Technol. B* **4**, 1055 (1986).
5. “Theoretical study of band offsets at semiconductor interfaces”, C. G. Van de Walle and R. M. Martin, *Phys. Rev. B* **35**, 8154 (1987). [doi: [10.1103/PhysRevB.35.8154](https://doi.org/10.1103/PhysRevB.35.8154)]
6. “Band offsets at interfaces between HgTe, CdTe, and InSb”, C. G. Van de Walle and R. M. Martin, *J. Vac. Sci. Technol. B* **5**, 1225 (1987).
7. “Strain and the interpretation of band-lineup measurements”, J. Tersoff and C. G. Van de Walle, *Phys. Rev. Lett.* **59**, 946 (1987).
8. “Comment on “Heterojunction valence-band-discontinuity dependence on face orientation” “ C. G. Van de Walle and R. M. Martin, *Phys. Rev. B* **37**, 4801 (1988).
9. “Theoretical investigations of fluorine-silicon systems”, C. G. Van de Walle, Y. Bar-Yam, F. R. McFeely, and S. T. Pantelides, *J. Vac. Sci. Technol. A* **6**, 1973 (1988).
10. “Theory of hydrogen diffusion and reactions in crystalline silicon”, C. G. Van de Walle, Y. Bar-Yam, and S. T. Pantelides, *Phys. Rev. Lett.* **60**, 2761 (1988). [doi: [10.1103/PhysRevLett.60.2761](https://doi.org/10.1103/PhysRevLett.60.2761)]
11. “Optical characterization and band offsets in $\text{ZnSe-ZnS}_x\text{Se}_{1-x}$ strained-layer superlattices”, K. Shahzad, D. J. Olego, and C. G. Van de Walle, *Phys. Rev. B* **38**, 1417 (1988); **43**, 1830 (1991) (E).
12. “Strained-layer interfaces between II-VI compound semiconductors”, C. G. Van de Walle, K. Shahzad, and D. J. Olego, *J. Vac. Sci. Technol. B* **6**, 1350 (1988).
13. “Fluorine-silicon reactions and the etching of crystalline silicon”, C. G. Van de Walle, F. R. McFeely, and S. T. Pantelides, *Phys. Rev. Lett.* **61**, 1867 (1988).

14. “Band lineups and deformation potentials in the model-solid theory”, C. G. Van de Walle, Phys. Rev. B **39**, 1871 (1989). [doi: [10.1103/PhysRevB.39.1871](https://doi.org/10.1103/PhysRevB.39.1871)]
15. “Mechanisms of equilibrium and nonequilibrium diffusion of dopants in silicon”, C. S. Nichols, C. G. Van de Walle, and S. T. Pantelides, Phys. Rev. Lett. **62**, 1049 (1989). [doi: [10.1103/PhysRevLett.62.1049](https://doi.org/10.1103/PhysRevLett.62.1049)]
16. “Electronic properties of the (100) Si/Ge strained-layer superlattices”, S. Satpathy, R. M. Martin, and C. G. Van de Walle, Phys. Rev. B **38**, 13237 (1988).
17. “Atomic and electronic structure of Si-Ge superlattices”, C. G. Van de Walle, Phys. Rev. Lett. **62**, 974 (1989).
18. “Structure and properties of hydrogen-impurity pairs in elemental semiconductors”, P. J. H. Denteneer, C. G. Van de Walle, and S. T. Pantelides, Phys. Rev. Lett. **62**, 1884 (1989).
19. “ “Absolute” deformation potentials: formulation and *ab initio* calculations for semiconductors”, C. G. Van de Walle and R. M. Martin, Phys. Rev. Lett. **62**, 2028 (1989).
20. “Theory of hydrogen diffusion and reactions in crystalline silicon”, C. G. Van de Walle, P. J. H. Denteneer, Y. Bar-Yam, and S. T. Pantelides, Phys. Rev. B **39**, 10791 (1989). [doi: [10.1103/PhysRevB.39.10791](https://doi.org/10.1103/PhysRevB.39.10791)]
21. “Microscopic structure of the hydrogen-boron complex in crystalline silicon”, P. J. H. Denteneer, C. G. Van de Walle, and S. T. Pantelides, Phys. Rev. B **39**, 10809 (1989).
22. “Microscopic structure of the hydrogen-phosphorous complex in crystalline silicon”, P. J. H. Denteneer, C. G. Van de Walle, and S. T. Pantelides, Phys. Rev. B **41** 3885 (1990) (RC).
23. “Properties of hydrogen in crystalline silicon under compression and tension”, C. S. Nichols, D. R. Clarke, and C. G. Van de Walle, Phys. Rev. Lett. **63**, 1090 (1989).
24. “Mechanisms of dopant impurity diffusion in silicon”, C. S. Nichols, C. G. Van de Walle, and S. T. Pantelides, Phys. Rev. B **40**, 5484 (1989).
25. “Structural identification of hydrogen and muonium centers in silicon: First-principles calculations of hyperfine parameters”, C. G. Van de Walle, Phys. Rev. Lett. **64**, 669 (1990).
26. “First-principles calculations of diffusion coefficients: hydrogen in silicon”, P. E. Blöchl, C. G. Van de Walle, and S. T. Pantelides, Phys. Rev. Lett. **64**, 1401 (1990).
27. “Effects of strain on the optical and vibrational properties of ZnSe-ZnS_xSe_{1-x} strained-layer superlattices”, K. Shahzad, D. J. Olego, C. G. Van de Walle, and D. A. Cammack, J. Lumin. **46**, 109 (1990).
28. “Theoretical aspects of hydrogen in crystalline semiconductors”, C. G. Van de Walle, Physica B **170**, 21 (1991).
29. “Role of native defects in wide band-gap semiconductors”, D. B. Laks, C. G. Van de Walle,

- G. F. Neumark, and S. T. Pantelides, Phys. Rev. Lett. **66**, 648 (1991).
30. “Atomic and electronic structure of CaSi₂/Si interfaces”, C. G. Van de Walle, Phys. Rev. B **43**, 11913 (1991).
 31. “Theory of defects, impurities, and doping in ZnSe”, C. G. Van de Walle and D. B. Laks, J. Lumin. **52**, 1 (1992).
 32. “Native defects and self-compensation in ZnSe”, D. B. Laks, C. G. Van de Walle, G. F. Neumark, P. E. Blöchl, and S. T. Pantelides, Phys. Rev. B **45**, 10965 (1992). [doi: [10.1103/PhysRevB.45.10965](https://doi.org/10.1103/PhysRevB.45.10965)]
 33. “First-principles calculations of solubilities and doping limits: Li, Na, and N in ZnSe”, C. G. Van de Walle, D. B. Laks, G. F. Neumark, and S. T. Pantelides, Phys. Rev. B **47**, 9425 (1993). [doi: [10.1103/PhysRevB.47.9425](https://doi.org/10.1103/PhysRevB.47.9425)]
 34. “Solubilities, defect reactions, and doping limits in ZnSe”, C. G. Van de Walle, D. B. Laks, G. F. Neumark, and S. T. Pantelides, J. Crystal Growth **117**, 704 (1992).
 35. “First-principles calculations of hyperfine parameters”, C. G. Van de Walle and P. E. Blöchl, Phys. Rev. B **47**, 4244 (1993). [doi: [10.1103/PhysRevB.47.4244](https://doi.org/10.1103/PhysRevB.47.4244)]
 36. “Spin-polarized calculations and hyperfine parameters for hydrogen and muonium in GaAs”, C. G. Van de Walle and L. Pavesi, Phys. Rev. B **47**, 4256 (1993).
 37. “Doping limits in ZnSe”, D. B. Laks and C. G. Van de Walle, Physica B **185**, 118 (1993).
 38. “First-principles investigation of visible light emission from silicon-based materials”, C. G. Van de Walle and J. E. Northrup, Phys. Rev. Lett. **70**, 1116 (1993).
 39. “Acceptor doping in ZnSe versus ZnTe”, D. B. Laks, C. G. Van de Walle, G. F. Neumark, and S. T. Pantelides, Appl. Phys. Lett. **63**, 1375 (1993).
 40. “Energies of various configurations of hydrogen in silicon”, C. G. Van de Walle, Phys. Rev. B **49**, 4579 (1994); *ibid.* **58**, 1689 (1998) (Erratum).
 41. “Structure, energetics, and dissociation of Si-H bonds at dangling bonds in silicon”, C. G. Van de Walle and R. A. Street, Phys. Rev. B **49**, 14 766 (1994) (RC). [doi: [10.1103/PhysRevB.49.14766](https://doi.org/10.1103/PhysRevB.49.14766)]
 42. “Silicon-hydrogen bonding and hydrogen diffusion in amorphous silicon”, C. G. Van de Walle and R. A. Street, Phys. Rev. B **51**, 10 615 (1995).
 43. “Hydrogen-induced metastable changes in the electrical conductivity of polycrystalline silicon”, N. H. Nickel, N. M. Johnson, and C. G. Van de Walle, Phys. Rev. Lett. **72**, 3393 (1994).
 44. “Energetics of bond-centered hydrogen in strained Si-Si bonds”, C. G. Van de Walle and N. H. Nickel, Phys. Rev. B **51**, 2636 (1995) (RC).

45. “Inverted order of acceptor and donor levels of monatomic hydrogen in silicon”, N. M. Johnson, C. Herring, and C. G. Van de Walle, *Phys. Rev. Lett.* **73**, 130 (1994); **74**, 1889 (1995) (erratum).
46. Comment on “Electron paramagnetic resonance of molecular hydrogen in silicon”, K. L. Brower, S. M. Myers, A. H. Edwards, N. M. Johnson, C. G. Van de Walle, and E. H. Poindexter, *Phys. Rev. Lett.* **73**, 1456 (1994).
47. “Atomic geometry and electronic structure of native defects in GaN”, J. Neugebauer and C. G. Van de Walle, *Phys. Rev. B* **50**, 8067 (1994) (RC). [doi: [10.1103/PhysRevB.50.8067](https://doi.org/10.1103/PhysRevB.50.8067)]
48. “Nitrogen doping in ZnTe and ZnSe”, C. G. Van de Walle and D. B. Laks, *Solid State Communications* **93**, 447 (1995).
49. “Electronic structure and phase stability of GaAs_{1-x}N_x alloys”, J. Neugebauer and C. G. Van de Walle, *Phys. Rev. B* **51**, 10 568 (1995).
50. “Band discontinuities at heterojunctions between crystalline and amorphous silicon”, C. G. Van de Walle and L. H. Yang, *J. Vac. Sci. Technol. B* **13**, 1635 (1995).
51. “Hydrogen in GaN: novel aspects of a common impurity”, J. Neugebauer and C. G. Van de Walle, *Phys. Rev. Lett.* **75**, 4452 (1995). [doi: [10.1103/PhysRevLett.75.4452](https://doi.org/10.1103/PhysRevLett.75.4452)]
52. “Native defects and impurities in GaN”, J. Neugebauer and C. G. Van de Walle, in *Festkörperprobleme/Advances in Solid State Physics*, Vol. **35**, ed. by R. Helbig (Vieweg, Braunschweig/Wiesbaden, 1996), p. 25.
53. Reply to “Comment on 'Inverted order of acceptor and donor levels of monatomic hydrogen in silicon'”, N. M. Johnson, C. Herring, and C. G. Van de Walle, *Phys. Rev. Lett.* **74**, 4566 (1995).
54. “'Stretched exponential' relaxation modeled without invoking statistical distributions”, C. G. Van de Walle, *Phys. Rev. B.* **53**, 11292 (1996).
55. “Defects, impurities and doping levels in wide-band-gap semiconductors”, C. G. Van de Walle and J. Neugebauer, *Brazilian Journal of Physics* **26**, 163 (1996).
56. “Hydrogen interactions with self-interstitials in silicon”, C. G. Van de Walle and J. Neugebauer, *Phys. Rev. B* **52**, R14 320 (1995) (RC). [doi: [10.1103/PhysRevB.52.R14320](https://doi.org/10.1103/PhysRevB.52.R14320)]
57. “Atomic arrangement at the AlN/SiC interface”, F. A. Ponce, C. G. Van de Walle, and J. E. Northrup, *Phys. Rev. B* **53**, 7473 (1996).
58. “Role of hydrogen in doping of GaN”, J. Neugebauer and C. G. Van de Walle, *Appl. Phys. Lett.* **68**, 1829 (1996). [doi: [10.1063/1.116027](https://doi.org/10.1063/1.116027)]
59. “Gallium vacancies and the yellow luminescence in GaN”, J. Neugebauer and C. G. Van de Walle, *Appl. Phys. Lett.* **69**, 503 (1996). [doi: [10.1063/1.117767](https://doi.org/10.1063/1.117767)]

60. "Comment on 'Reduction of hot electron degradation in metal oxide semiconductor transistors by deuterium processing' ", C. G. Van de Walle and W. B. Jackson, *Appl. Phys. Lett.* **69**, 2441 (1996). [doi: [10.1063/1.117664](https://doi.org/10.1063/1.117664)]
61. "Clean and As-covered zinc-blende GaN (001) surfaces: novel structures and surfactant behavior", J. Neugebauer, T. Zywiec, M. Scheffler, J. E. Northrup, and C. G. Van de Walle, *Phys. Rev. Lett.* **80**, 3097 (1998).
62. "Comment on " Surface silicon-deuterium bond energy from gas-phase equilibration", C. Herring and C. G. Van de Walle, *Phys. Rev. B.* **55**, 13 314 (1997).
63. "Small valence-band offsets at GaN/InGaN heterojunctions", C. G. Van de Walle and J. Neugebauer, *Appl. Phys. Lett.* **70**, 2577 (1997).
64. "Defects and doping in GaN", C. G. Van de Walle, *Braz. J. Phys.* **27/A**, 74 (1997).
65. "Interactions of hydrogen with native defects in GaN", C. G. Van de Walle, *Phys. Rev. B* **56**, R10 020 (1997).
66. "Hydrogen states in silicon", C. G. Van de Walle, *J. Non-Cryst. Solids* **227-230**, 111 (1998).
67. "DX center formation in wurtzite and zinc-blende AlGa_xN", C. G. Van de Walle, *Phys. Rev. B* **57**, 2033 (1998).
68. "Energetics and vibrational frequencies of interstitial H₂ molecules in semiconductors", C. G. Van de Walle, *Phys. Rev. Lett.* **80**, 2177 (1998).
69. "Doping of Al_xGa_{1-x}N", C. Stampfl and C. G. Van de Walle, *Appl. Phys. Lett.* **72**, 459 (1998).
70. "Theory of doping and defects in III-V nitrides", C. G. Van de Walle, C. Stampfl, and J. Neugebauer, *J. Cryst. Growth* **189/190**, 505 (1998).
71. "Chemical trends for acceptor impurities in GaN", J. Neugebauer and C. G. Van de Walle, *J. Appl. Phys.* **85**, 3003 (1999).
72. "Hydrogen in silicon: fundamental properties and consequences for devices", C. G. Van de Walle, *J. Vac. Sci. Technol. A* **16**, 1767 (1998).
73. "Energetics and electronic structure of stacking faults in AlN, GaN, and InN", C. Stampfl and C. G. Van de Walle, *Phys. Rev. B* **57**, R15052 (1998).
74. "Metastability of oxygen donors in AlGa_xN", M. D. McCluskey, N. M. Johnson, C. G. Van de Walle, D. P. Bour, M. Kneissl, and W. Walukiewicz, *Phys. Rev. Lett.* **80**, 4008 (1998).

75. “Characteristics of InGaN/AlGaIn multiple quantum well laser diodes”, D. P. Bour, M. Kneissl, L. T. Romano, M. McCluskey, C. G. Van de Walle, B. S. Krusor, R. Donaldson, J. Walker, C. Dunnrowicz, and N. M. Johnson, *IEEE J. Select. Topics Quantum Electron.* **4**, 498 (1998).
76. “Large band-gap bowing of $\text{In}_x\text{Ga}_{1-x}\text{N}$ alloys”, M. D. McCluskey, C. G. Van de Walle, C. P. Master, L. T. Romano, and N. M. Johnson, *Appl. Phys. Lett.* **72**, 2725 (1998).
77. “Surface structures, surfactants and diffusion at cubic and wurtzite GaN”, T. K. Zywietz, J. Neugebauer, M. Scheffler, J. E. Northrup, and C. G. Van de Walle, *MRS Internet Journal for Nitride Research* **3**, 26 (1998).
78. “First-principles study of native point defects in ZnO”, A. F. Kohan, G. Ceder, D. Morgan, and C. G. Van de Walle, *Phys. Rev. B* **61**, 15019 (2000).
79. “Exchange of deeply trapped and interstitial hydrogen in silicon”, B. Tuttle, C. G. Van de Walle, and J. B. Adams, *Phys. Rev. B* **59**, 5493 (1999).
80. “MOCVD growth and characterization of AlGaInN multiple quantum well heterostructures and laser diodes”, D. P. Bour, M. Kneissl, D. Hofstetter, L. T. Romano, M. McCluskey, C. G. Van de Walle, B. S. Krusor, C. Dunnrowicz, R. Donaldson, J. Walker, and N. M. Johnson, *Materials Science and Engineering B* **59**, 33 (1999).
81. “Doping of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys”, C. Stampfl, J. Neugebauer, and C. G. Van de Walle, *Materials Science and Engineering B* **59**, 253 (1999).
82. “Large and composition-dependent band-gap bowing in $\text{In}_x\text{Ga}_{1-x}\text{N}$ alloys”, C. G. Van de Walle, M. D. McCluskey, C. P. Master, L. T. Romano, and N. M. Johnson, *Materials Science and Engineering B* **59**, 274 (1999).
83. “Energetics and vibrational frequencies of interstitial H_2 molecules in semiconductors”, C. G. Van de Walle and J. Goss, *Materials Science and Engineering B* **58**, 17 (1999).
84. “Structure, energetics, and vibrational properties of Si-H bond dissociation in silicon”, B. Tuttle and C. G. Van de Walle, *Phys. Rev. B.* **59**, 12884 (1999). [doi: [10.1103/PhysRevB.59.12884](https://doi.org/10.1103/PhysRevB.59.12884)]
85. “Density-functional calculations for III-V nitrides using the local density approximation and the generalized gradient approximation”, C. Stampfl and C. G. Van de Walle, *Phys. Rev. B* **59**, 5521 (1999). [doi: [10.1103/PhysRevB.59.5521](https://doi.org/10.1103/PhysRevB.59.5521)]
86. “Native defects and impurities in InN: First-principles studies using the local-density approximation and self-interaction and relaxation-corrected pseudopotentials”, C. Stampfl, C. G. Van de Walle, D. Vogel, P. Krüger, and J. Pollmann, *Phys. Rev. B* **61**, R7846 (2000).
87. “DX centers in AlGaIn”, M. D. McCluskey, C. G. Van de Walle, N. M. Johnson, D. P. Bour, and M. Kneissl, *Int. J. Modern Physics B* **13**, 1363 (1999).

88. "Defects and defect reactions in semiconductor nitrides", C. G. Van de Walle, J. Neugebauer, C. Stampfl, M. D. McCluskey, and N. M. Johnson, *Acta Physica Polonica A* **96**, 613 (1999).
89. "Room-temperature continuous-wave operation of InGaN multiple quantum well laser diodes with an asymmetric waveguide structure", M. Kneissl, D. P. Bour, C. G. Van de Walle, L. T. Romano, J. E. Northrup, R. M. Wood, M. Teepe, and N. M. Johnson, *Appl. Phys. Lett.* **75**, 581 (1999).
90. "Arsenic impurities in GaN", C. G. Van de Walle and J. Neugebauer, *Appl. Phys. Lett.* **76**, 1009 (2000).
91. "Room-temperature continuous-wave operation of InGaN multiple quantum well laser diodes with an asymmetric waveguide structure", M. Kneissl, D. P. Bour, C. G. Van de Walle, L. T. Romano, J. E. Northrup, R. M. Wood, M. Teepe, T. Schmidt, and N. M. Johnson, *phys. stat. sol. (a)* **176**, 49 (1999).
92. "Design and performance of asymmetric waveguide nitride laser diodes", D. P. Bour, M. Kneissl, C. G. Van de Walle, G. A. Evans, L. T. Romano, J. E. Northrup, M. Teepe, R. M. Wood, T. Schmidt, and N. M. Johnson, *IEEE J. Quantum Electron.* **36**, 184 (2000).
93. "Performance and optical gain characteristic of InGaN MQW laser diodes", M. Kneissl, C. G. Van de Walle, D. P. Bour, L. T. Romano, L. L. Goddard, C. P. Master, J. E. Northrup, and N. M. Johnson, *Journal of Luminescence* **87-89**, 135 (2000).
94. "Effect of Si doping on the strain and defect structure of GaN thin films", L. T. Romano, C. G. Van de Walle, B. S. Krusor, R. Lau, J. Ho, T. Schmidt, J. W. Ager III, W. Götz, and R. S. Kern, *Physica B* **273-274**, 50 (1999).
95. "Microscopic theory of hydrogen in silicon devices", C. G. Van de Walle and B. Tuttle, *IEEE Trans. Electron Dev.* **47**, 1779 (2000). [doi: [10.1109/16.870547](https://doi.org/10.1109/16.870547)]
96. "Phase separation in InGaN multiple quantum wells annealed at high nitrogen pressures", L.T. Romano, M. D. McCluskey, C. G. Van de Walle, J. E. Northrup, D. P. Bour, M. Kneissl, T. Suski, and J. Jun, *Appl. Phys. Lett.* **75**, 3950 (1999).
97. "Hydrogen as a cause of doping in ZnO", C. G. Van de Walle, *Phys. Rev. Lett.* **85**, 1012 (2000). [doi: [10.1103/PhysRevLett.85.1012](https://doi.org/10.1103/PhysRevLett.85.1012)]
98. "The effect of Si doping on strain, cracking, and microstructure in GaN thin films grown by metalorganic chemical vapor deposition", L. T. Romano, C. G. Van de Walle, J. W. Ager III, W. Götz, and R. S. Kern, *J. Appl. Phys.* **87**, 7745 (2000).
99. "Polycrystalline nitride semiconductor light-emitting diodes fabricated on quartz substrates", D. P. Bour, N. M. Nickel, C. G. Van de Walle, M. S. Kneissl, B. S. Krusor, Ping Mei, and N. M. Johnson, *Appl. Phys. Lett.* **76**, 2182 (2000).

100. "Performance and degradation of continuous-wave InGaN multiple-quantum-well laser diodes on epitaxially laterally overgrown GaN substrates", M. Kneissl, D. P. Bour, L. T. Romano, C. G. Van de Walle, J. E. Northrup, W. S. Wong, D. W. Treat, M. Teepe, T. Schmidt, and N. M. Johnson, *Appl. Phys. Lett.* **77**, 1931 (2000).
101. "Magnesium incorporation in GaN grown by molecular-beam epitaxy", A. J. Ptak, T. H. Myers, L. T. Romano, C. G. Van de Walle, and J. E. Northrup, *Appl. Phys. Lett.* **78**, 285 (2001).
102. "First-principles studies of beryllium doping of GaN", C. G. Van de Walle, S. Limpijumnong, and J. Neugebauer, *Phys. Rev. B* **63**, 245205 (2001).
103. "Energy levels of isolated interstitial hydrogen in silicon", C. Herring, N. M. Johnson, and C. G. Van de Walle, *Phys. Rev. B* **64**, 125209 (2001).
104. "Entropy-driven stabilization of a novel configuration for acceptor-hydrogen complexes in GaN", S. Limpijumnong, C. G. Van de Walle, and J. E. Northrup, *Phys. Rev. Lett.* **87**, 205505 (2001).
105. "Influence of microstructure on the carrier concentration of Mg-doped GaN films", L. T. Romano, M. Kneissl, J. E. Northrup, C. G. Van de Walle, and D. W. Treat, *Appl. Phys. Lett.* **79**, 2734 (2001).
106. "First-principles surface phase diagram for hydrogen on GaN surfaces", C. G. Van de Walle and J. Neugebauer, *Phys. Rev. Lett.* **88**, 066103 (2002).
107. "Passivation and doping due to hydrogen in III-nitrides", S. Limpijumnong and C. G. Van de Walle, *phys. stat. sol. (b)* **228**, 303 (2001).
108. "Strategies for controlling the conductivity of wide-band-gap semiconductors", C. G. Van de Walle, *phys. stat. sol. (b)* **229**, 221 (2002).
109. "Defect analysis and engineering in ZnO", C. G. Van de Walle, *Physica B* **308-310**, 899 (2001).
110. "Theoretical investigation of native defects, impurities and complexes in AlN", C. Stampfl and C. G. Van de Walle, *Phys. Rev. B* **65**, 155212 (2002).
111. "Identification of hydrogen configurations in *p*-type GaN through first-principles calculations of vibrational frequencies", S. Limpijumnong, J. E. Northrup, and C. G. Van de Walle, *Phys. Rev. B* **68**, 075206 (2003).
112. "Band gap changes of GaN shocked to 13 GPa", M. D. McCluskey, Y. M. Gupta, C. G. Van de Walle, D. P. Bour, M. Kneissl, and N. M. Johnson, *Appl. Phys. Lett.* **80**, 1912 (2002).
113. "Quantitative analysis of the polarization fields and absorption changes in InGaN/GaN quantum wells with electroabsorption spectroscopy", F. Renner, P. Kiesel, G. H. Döhler,

- M. Kneissl, C. Van de Walle, and N. M. Johnson, *Appl. Phys. Lett.* **81**, 490 (2002).
114. “Role of hydrogen in surface reconstructions and growth of GaN”, C. G. Van de Walle and J. Neugebauer, *J. Vac. Sci. Technol. B* **20**, 1640 (2002).
115. “Effects of hydrogen on the electronic properties of dilute GaAsN alloys”, A. Janotti, S. B. Zhang, Su-Huai Wei, and C. G. Van de Walle, *Phys. Rev. Lett.* **89**, 086403 (2002).
116. “Hydrogen-related defects in ZnO studied by infrared absorption spectroscopy”, E. V. Lavrov, J. Weber, F. Börrnert, C. G. Van de Walle, and R. Helbig, *Phys. Rev. B* **66**, 165205 (2002).
117. “Structure and energetics of nitride surfaces under MOCVD growth conditions”, C. G. Van de Walle and J. Neugebauer, *J. Cryst. Growth* **248**, 8 (2003).
118. “Hydrogen as a shallow center in semiconductors and oxides”, C. G. Van de Walle, *phys. stat. sol. (b)* **235**, 89 (2003).
119. “Shallow donor state of hydrogen in indium nitride”, E. A. Davis, S. F. J. Cox, R. L. Lichti, and C. G. Van de Walle, *Appl. Phys. Lett.* **82**, 592 (2003).
120. “Physics and chemistry of hydrogen in the vacancies of semiconductors”, B. Szűcs, A. Gali, Z. Hajnal, P. Deák, and C. G. Van de Walle, *Phys. Rev. B* **68**, 085202 (2003).
121. “Quantitative analysis of absorption and field-induced absorption changes in InGaN/GaN quantum wells”, P. Kiesel, F. Renner, M. Kneissl, C. Van de Walle, G. H. Döhler, and N. M. Johnson, *phys. stat. sol.* **234**, 742 (2002).
122. “Effect of composition on the band gap of strained $\text{In}_x\text{Ga}_{1-x}\text{N}$ alloys”, M. D. McCluskey, C. G. Van de Walle, L. T. Romano, B. S. Krusor, and N. M. Johnson, *J. Appl. Phys.* **93**, 4340 (2003).
123. “Universal alignment of hydrogen levels in semiconductors, insulators and solutions”, C. G. Van de Walle and J. Neugebauer, *Nature* **423**, 626 (2003). [doi: [10.1038/nature01665](https://doi.org/10.1038/nature01665)]
124. “Interactions between nitrogen, hydrogen, and gallium vacancies in GaAsN alloys”, A. Janotti, S. Wei, S. Zhang, S. Kurtz, and C. G. Van de Walle, *Phys. Rev. B* **67**, 161201 (2003).
125. “Electronic materials theory: Interfaces and defects”, C. G. Van de Walle, *J. Vac. Sci. Technol. A* **21**, S182 (2003).
126. “Effects of impurities on the lattice parameters of GaN”, C. G. Van de Walle, *Phys. Rev. B* **68**, 165209 (2003).
127. “Stability, diffusivity, and vibrational properties of interstitial hydrogen in wurtzite GaN”, S. Limpijumnong and C. G. Van de Walle, *Phys. Rev. B* **68**, 235203 (2003). [doi: [10.1103/PhysRevB.68.235203](https://doi.org/10.1103/PhysRevB.68.235203)]

128. "Diffusivity of native defects in GaN", S. Limpijumnong and C. G. Van de Walle, Phys. Rev. B **69**, 035207 (2004). [doi: [10.1103/PhysRevB.69.035207](https://doi.org/10.1103/PhysRevB.69.035207)]
129. "Effects of N on the electronic structures of H defects in III-V semiconductors", A. Janotti, S. B. Zhang, Su-Huai Wei, and C. G. Van de Walle, Optical Materials **25**, 261 (2004).
130. "Indium versus hydrogen-terminated GaN(0001) surfaces: Surfactant effect of indium in a chemical vapor deposition environment", J. E. Northrup and C. G. Van de Walle, Appl. Phys. Lett. **84**, 4322 (2004).
131. "Hydrogen passivation effect in nitrogen-doped ZnO thin films", X. Li, B. Keyes, S. Asher, S. B. Zhang, S.-H. Wei, T. J. Coutts, S. Limpijumnong, and C. G. Van de Walle, Appl. Phys. Lett. **86**, 122107 (2005).
132. "Oxygen vacancies in ZnO", A. Janotti and C. G. Van de Walle, Appl. Phys. Lett. **87**, 122102 (2005). [doi: [10.1063/1.2053360](https://doi.org/10.1063/1.2053360)]
133. "Evidence for an electrically conducting layer at the native zinc oxide surface", O. Schmidt, P. Kiesel, C. G. Van de Walle, N. M. Johnson, J. Nause, and G. H. Döhler, Jpn. J. Appl. Phys. Part 1 **44**, 7271 (2005).
134. "New insights into the role of native point defects in ZnO", A. Janotti and C. G. Van de Walle, J. Cryst. Growth **287**, 58-65 (2006).
135. "Analysis of a conducting channel at the native zinc oxide surface", O. Schmidt, A. Geis, P. Kiesel, C. G. Van de Walle, N. M. Johnson, A. Bakin, A. Waag, and G. H. Döhler, Superlatt. Microstructur. **39**, 8 (2006).
136. "Universal alignment of hydrogen levels in semiconductors and insulators", C. G. Van de Walle, Physica B **376-377**, 1 (2006).
137. "Effects of cation d states on the structural and electronic properties of III-nitride and II-oxide wide-band-gap semiconductors", A. Janotti, D. Segev, and C. G. Van de Walle, Phys. Rev. B **74**, 045202 (2006).
138. "Origins of Fermi-level pinning on GaN and InN polar and nonpolar surfaces", D. Segev and C. G. Van de Walle, Europhys. Lett. **76**, 305 (2006).
139. "Hydrogen multicenter bonds", A. Janotti and C. G. Van de Walle, Nature Materials **6**, 44 (2007). [doi: [10.1038/nmat1795](https://doi.org/10.1038/nmat1795)]
140. "Self-consistent band-gap corrections in density functional theory using modified pseudopotentials", D. Segev, A. Janotti, and C. G. Van de Walle, Phys. Rev. B **75**, 035201 (2007).
141. "Surface reconstructions on InN and GaN polar and nonpolar surfaces", D. Segev and C. G. Van de Walle, Surf. Sci. **601**, L15 (2007).
142. "Electronic structure of nitride surfaces", D. Segev and C. G. Van de Walle, J. Cryst. Growth **300**, 199 (2007).

143. "Absolute deformation potentials and band alignment of wurtzite ZnO, MgO, and CdO", A. Janotti and C. G. Van de Walle, Phys. Rev. B **75**, 121201 (2007).
144. "Microscopic origins of surface states on nitride surfaces", C. G. Van de Walle and D. Segev, J. Appl. Phys. **101**, 081704 (2007).
145. "Native Point Defects in ZnO", A. Janotti and C. G. Van de Walle, Phys. Rev. B **76**, 165202 (2007). [doi: [10.1103/PhysRevB.76.165202](https://doi.org/10.1103/PhysRevB.76.165202)]
146. "Dangling-bond defects and hydrogen passivation in germanium", J. Weber, A. Janotti, P. Rinke, and C. G. Van de Walle, Appl. Phys. Lett. **91**, 142101 (2007). [doi: [10.1063/1.2793184](https://doi.org/10.1063/1.2793184)]
147. "Hydrogen in semiconductors and insulators", C. G. Van de Walle, J. Alloys Compd. **446-448**, 48 (2007).
148. "Hydrogen-related defects in sodium alanate", A. Peles and C. G. Van de Walle, J. Alloys Compd. **446-447**, 459 (2007).
149. "Role of charged defects and impurities in kinetics of hydrogen storage materials: A first-principles study", A. Peles and C. G. Van de Walle, Phys. Rev. B **76**, 214101 (2007). [doi: [10.1103/PhysRevB.76.214101](https://doi.org/10.1103/PhysRevB.76.214101)]
150. "Sources of unintentional *n*-type conductivity in InN", A. Janotti and C. G. Van de Walle, Appl. Phys. Lett. **92**, 032104 (2008).
151. "Computational studies of conductivity in wide-band-gap semiconductors and oxides", C. G. Van de Walle, J. Phys.: Condens. Matter **20**, 064230 (2008).
152. "Optimizing Optical Absorption of TiO₂ by Alloying with TiS₂", N. Umezawa, A. Janotti, P. Rinke, T. Chikyow, and C. G. Van de Walle, Appl. Phys. Lett. **92**, 041104 (2008).
153. "Mutual Passivation of Electrically Active and Isovalent Impurities in Dilute Nitrides", A. Janotti, P. Reunchan, S. Limpijumnong, and C. G. Van de Walle, Phys. Rev. Lett. **100**, 045505 (2008).
154. "Near-infrared absorption and semimetal-semiconductor transition in 2 nm ErAs nanoparticles embedded in GaAs and AlAs", M. A. Scarpulla, J. M. O. Zide, J. M. LeBeau, C. G. Van de Walle, A. C. Gossard, and K. T. Delaney, Appl. Phys. Lett. **92**, 173116 (2008).
155. "Carbon-nitrogen molecules in GaAs and GaP", S. Limpijumnong, P. Reunchan, A. Janotti, and C. G. Van de Walle, Phys. Rev. B **77**, 195209 (2008).
156. "Theoretical study of the structural and electronic properties of strained ErAs", K. T. Delaney, N. A. Spaldin, and C. G. Van de Walle, Phys. Rev. B **77**, 235117 (2008).
157. "Sources of Electrical Conductivity in SnO₂", A. K. Singh, A. Janotti, M. Scheffler, and C. G. Van de Walle, Phys. Rev. Lett. **101**, 055502 (2008).

158. “Electrical activity of hydrogen impurities in GaSb: First-principles calculations”, A. Peles, A. Janotti, and C. G. Van de Walle, *Phys. Rev. B* **78**, 035204 (2008).
159. “Step-flow growth of ZnO(0001) on GaN(0001) by metalorganic chemical vapor epitaxy”, T. Ive, T. Ben-Yaacov, C. G. Van de Walle, U. K. Mishra, S. P. DenBaars, and J. S. Speck, *J. Cryst. Growth* **310**, 3407 (2008).
160. “Role of hydrogen at germanium/dielectric interfaces”, C. G. Van de Walle, J. R. Weber, and A. Janotti, *Thin Solid Films* **517**, 144 (2008).
161. “Causes of incorrect carrier-type identification in van der Pauw–Hall measurements”, O. Bierwagen, T. Ive, C. G. Van de Walle, and J. S. Speck, *Appl. Phys. Lett.* **93**, 242108 (2008).
162. “Fully *ab initio* finite-size corrections for charged-defect supercell calculations”, C. Freysoldt, J. Neugebauer, and C G. Van de Walle, *Phys. Rev. Lett.* **102**, 016402 (2009). [doi: [10.1103/PhysRevLett.102.016402](https://doi.org/10.1103/PhysRevLett.102.016402)]
163. “Defect Formation Energies without the Band-Gap Problem: Combining Density-Functional Theory and the GW Approach for the Silicon Self-Interstitial”, P. Rinke, A. Janotti, M. Scheffler, and C. G. Van de Walle, *Phys. Rev. Lett.* **102**, 026402 (2009).
164. “Role of Atomic Multiplets in the Electronic Structure of Rare-Earth Semiconductors and Semimetals”, L. V. Pourovskii, K. T. Delaney, C. G. Van de Walle, N. A. Spaldin, and A. Georges, *Phys. Rev. Lett.* **102**, 096401 (2009).
165. “Atomic and electronic structure of hydrogen-related centers in hydrogen storage materials”, C. G. Van de Walle, A. Peles, A. Janotti, and G. B. Wilson-Short, *Physica B* **404**, 793 (2009).
166. “Dissipation-factor-based criterion for the validity of carrier-type identification by capacitance-voltage measurements”, O. Bierwagen, T. Nagata, T. Ive, C. G. Van de Walle, and J. S. Speck, *Appl. Phys. Lett.* **94**, 152110 (2009).
167. “Auger recombination rates in nitrides from first principles”, K. T. Delaney, P. Rinke, and C. G. Van de Walle, *Appl. Phys. Lett.* **94**, 191109 (2009); **108**, 259901 (2016) (erratum).
168. “Hydrogen interactions with acceptor impurities in SnO₂: First-principles calculations”, J. B. Varley, A. Janotti, A. K. Singh, and C. G. Van de Walle, *Phys. Rev. B* **79**, 245206 (2009).
169. “Point defects in Al₂O₃ and their impact on gate stacks”, J. R. Weber, A. Janotti and C. G. Van de Walle, *Microel. Eng.* **86**, 1756 (2009). [doi: [10.1016/j.mee.2009.03.059](https://doi.org/10.1016/j.mee.2009.03.059)]
170. “Formation and migration of charged native point defects in MgH₂: First-principles calculations”, M. S. Park, A. Janotti, and C. G. Van de Walle, *Phys. Rev. B* **80**, 064102 (2009).

171. “First-principles investigations of F and Cl impurities in NaAlH₄”, G. B. Wilson-Short, A. Janotti, A. Peles, and C. G. Van de Walle, *J. Alloys Compd.* **484**, 347 (2009). [[doi:10.1016/j.jallcom.2009.04.091](https://doi.org/10.1016/j.jallcom.2009.04.091)]
172. “Strain effects in group-III nitrides: Deformation potentials for AlN, GaN, and InN”, Q. Yan, P. Rinke, M. Scheffler, and C. G. Van de Walle, *Appl. Phys. Lett.* **95**, 121111 (2009). [[doi: 10.1063/1.3236533](https://doi.org/10.1063/1.3236533)]
173. “Hydrogen doping in indium oxide: An *ab initio* study”, S. Limpijumnong, P. Reunchan, A. Janotti, and C. G. Van de Walle, *Phys. Rev. B* **80**, 193202 (2009). [[doi: 10.1103/PhysRevB.80.193202](https://doi.org/10.1103/PhysRevB.80.193202)]
174. “Interactions between hydrogen impurities and vacancies in Mg and Al: A comparative analysis based on density functional theory”, L. Ismer, M. S. Park, A. Janotti, and C. G. Van de Walle, *Phys. Rev. B* **80**, 184110 (2009) [[doi: 10.1103/PhysRevB.80.184110](https://doi.org/10.1103/PhysRevB.80.184110)]; *ibid.* **81**, 139902 (2010) (erratum).
175. “A pathway to *p*-type wide-band-gap semiconductors”, A. Janotti, E. Snow, and C. G. Van de Walle, *Appl. Phys. Lett.* **95**, 172109 (2009). [[doi:10.1063/1.3247890](https://doi.org/10.1063/1.3247890)]
176. “Reconstructions and origin of surface states on AlN polar and nonpolar surfaces”, M. S. Miao, A. Janotti, and C. G. Van de Walle, *Phys. Rev. B* **80**, 155319 (2009). [[doi: 10.1103/PhysRevB.80.155319](https://doi.org/10.1103/PhysRevB.80.155319)]
177. “First-principles study of the formation and migration of native defects in NaAlH₄”, G. B. Wilson-Short, A. Janotti, K. Hoang, A. Peles, and C. G. Van de Walle, *Phys. Rev. B* **80**, 224102 (2009). [[doi: 10.1103/PhysRevB.80.224102](https://doi.org/10.1103/PhysRevB.80.224102)]
178. “Hydrogen-related defects and the role of metal additives in the kinetics of complex hydrides: A first-principles study”, K. Hoang and C. G. Van de Walle, *Phys. Rev. B* **80**, 214109 (2009). [[doi: 10.1103/PhysRevB.80.214109](https://doi.org/10.1103/PhysRevB.80.214109)]
179. “Why nitrogen cannot lead to *p*-type conductivity in ZnO”, J. L. Lyons, A. Janotti, and C. G. Van de Walle, *Appl. Phys. Lett.* **95**, 252105 (2009). [[doi: 10.1063/1.3274043](https://doi.org/10.1063/1.3274043)]
180. “Role of Si and Ge as impurities in ZnO”, J. L. Lyons, A. Janotti, and C. G. Van de Walle, *Phys. Rev. B* **80**, 205113 (2009). [[doi: 10.1103/PhysRevB.80.205113](https://doi.org/10.1103/PhysRevB.80.205113)]
181. “Band bowing and band alignment in InGaN alloys”, P. G. Moses and C. G. Van de Walle, *Appl. Phys. Lett.* **96**, 021908 (2010). [[doi:10.1063/1.3291055](https://doi.org/10.1063/1.3291055)]
182. “Hybrid functional studies of the oxygen vacancy in TiO₂”, A. Janotti, J. B. Varley, P. Rinke, N. Umezawa, G. Kresse, and C. G. Van de Walle, *Phys. Rev. B* **81**, 085212 (2010). [[doi: 10.1103/PhysRevB.81.085212](https://doi.org/10.1103/PhysRevB.81.085212)]
183. “Effects of surface reconstructions on oxygen adsorption at AlN polar surfaces”, M. S. Miao, P. G. Moses, J. R. Weber, A. Janotti, and C. G. Van de Walle, *EuroPhys. Lett.* **89**, 56004 (2010). [[doi: 10.1209/0295-5075/89/56004](https://doi.org/10.1209/0295-5075/89/56004)]

184. “Origin and passivation of fixed charge in atomic layer deposited aluminum oxide gate insulators on chemically treated InGaAs substrates”, B. Shin, J. R. Weber, R. D. Long, P. K. Hurley, C. G. Van de Walle, and P. C. McIntyre, *Appl. Phys. Lett.* **96**, 152908 (2010).
185. “Theoretical study of Schottky-barrier formation at epitaxial rare-earth-metal/semiconductor interfaces”, K. T. Delaney, N. A. Spaldin, and C. G. Van de Walle, *Phys. Rev. B* **81**, 165312 (2010). [doi: [10.1103/PhysRevB.81.165312](https://doi.org/10.1103/PhysRevB.81.165312)]
186. “Controlling the conductivity of InN”, C. G. Van de Walle, J. L. Lyons, and A. Janotti, *Phys. Status Solidi A* **207**, 1024 (2010). [doi: [10.1002/pssa.200983122](https://doi.org/10.1002/pssa.200983122)]
187. “Properties of In-Doped ZnO Films Grown by Metalorganic Chemical Vapor Deposition on GaN(0001) Templates”, T. Ben-Yaacov, T. Ive, C. G. Van de Walle, U. K. Mishra, J. S. Speck, and S. P. DenBaars, *J. Electron. Mater.* **39**, 608 (2010). [doi: [10.1007/s11664-009-1022-x](https://doi.org/10.1007/s11664-009-1022-x)]
188. “Free-carrier absorption in nitrides from first principles”, E. Kioupakis, P. Rinke, A. Schleife, F. Bechstedt, and C. G. Van de Walle, *Phys. Rev. B* **81**, 241201 (2010). [doi: [10.1103/PhysRevB.81.241201](https://doi.org/10.1103/PhysRevB.81.241201)]
189. “Quantum Computing with Defects”, J. R. Weber, W. F. Koehl, J. B. Varley, A. Janotti, B. B. Buckley, C. G. Van de Walle, and D. D. Awschalom, *Proc. Nat. Acad. Sci.* **107**, 8513 (2010). [doi: [10.1073/pnas.1003052107](https://doi.org/10.1073/pnas.1003052107)]
190. “Oxidation and the origin of the two-dimensional electron gas in AlGaIn/GaN heterostructures”, M. S. Miao, J. R. Weber, and C. G. Van de Walle, *J. Appl. Phys.* **107**, 123713 (2010). [doi: [10.1063/1.3431391](https://doi.org/10.1063/1.3431391)]
191. “Determination of Internal Loss in Nitride Lasers from First Principles”, E. Kioupakis, P. Rinke, and C. G. Van de Walle, *Appl. Phys. Express* **3**, 082101 (2010). [doi: [10.1143/APEX.3.082101](https://doi.org/10.1143/APEX.3.082101)]
192. “Group-V impurities in SnO₂ from first-principles calculations”, J. B. Varley, A. Janotti, and C. G. Van de Walle, *Phys. Rev. B* **81**, 245216 (2010). [doi: [10.1103/PhysRevB.81.245216](https://doi.org/10.1103/PhysRevB.81.245216)]
193. “Alternative sources of *p*-type conduction in acceptor-doped ZnO”, S. Limpijumnong, L. Gordon, M. Miao, A. Janotti, and C. G. Van de Walle, *Appl. Phys. Lett.* **97**, 072112 (2010). [doi: [10.1063/1.3481069](https://doi.org/10.1063/1.3481069)]
194. “Distribution of donor states on etched surface of AlGaIn/GaN heterostructures”, M. Higashiwaki, S. Chowdhury, M. S. Miao, B. L. Swenson, C. G. Van de Walle, and U. K. Mishra, *J. Appl. Phys.* **108**, 063719 (2010). [doi: [10.1063/1.3481412](https://doi.org/10.1063/1.3481412)]
195. “Oxygen vacancies and donor impurities in β -Ga₂O₃”, J. B. Varley, J. R. Weber, A. Janotti, and C. G. Van de Walle, *Appl. Phys. Lett.* **97**, 142106 (2010). [doi: [10.1063/1.3499306](https://doi.org/10.1063/1.3499306)]
196. “Carbon impurities and the yellow luminescence in GaN”, J. L. Lyons, A. Janotti, and C. G. Van de Walle, *Appl. Phys. Lett.* **97**, 152108 (2010). [doi: [10.1063/1.3492841](https://doi.org/10.1063/1.3492841)]

197. “Hydrogen donors in SnO₂ studied by infrared spectroscopy and first-principles calculations”, W. M. Hlaing Oo, S. Tabatabaei, M. D. McCluskey, J. B. Varley, A. Janotti, and C. G. Van de Walle, Phys. Rev. B **82**, 193201 (2010). [doi: 10.1103/PhysRevB.82.193201]
198. “Role of strain in polarization switching in semipolar InGaN/GaN quantum wells”, Q. Yan, P. Rinke, M. Scheffler, and C. G. Van de Walle, Appl. Phys. Lett. **97**, 181102 (2010). [doi: 10.1063/1.3507289]
199. “Intrinsic and extrinsic causes of electron accumulation layers on InAs surfaces”, J. R. Weber, A. Janotti, and C. G. Van de Walle, Appl. Phys. Lett. **97**, 192106 (2010). [doi:10.1063/1.3518061]
200. “The electronic structure of β -Ga₂O₃”, M. Mohamed, C. Janowitz, I. Unger, R. Manzke, Z. Galazka, R. Uecker, R. Fornari, J. R. Weber, J. B. Varley, and C. G. Van de Walle, Appl. Phys. Lett. **97**, 211903 (2010). [doi:10.1063/1.3521255]
201. “Point-defect-mediated dehydrogenation of AlH₃”, L. Ismer, A. Janotti, and C. G. Van de Walle, Appl. Phys. Lett. **97**, 201902 (2010). [doi:10.1063/1.3518475]
202. “Vibrational signatures of O_{Te} and OT_e-V_{Cd} in CdTe: A first-principles study”, J. T-Thienprasert, S. Limpijumnong, A. Janotti, C. G. Van de Walle, L. Zhang, M. H. Du, and D. J. Singh, Comput. Mater. Sci. **49**, S242 (2010).
203. “Distributed surface donor states and the two-dimensional electron gas at AlGaN/GaN heterojunctions”, L. Gordon, M. S. Miao, S. Chowdhury, M. Higashiwaki, U. K. Mishra, and C. G. Van de Walle, J. Phys. D **43**, 505501 (2010). [doi: 10.1088/0022-3727/43/50/505501]
204. “Band parameters and strain effects in ZnO and group-III nitrides”, Q. Yan, P. Rinke, M. Winkelkemper, A. Qteish, D. Bimberg, M. Scheffler, and C. G. Van de Walle, Semicond. Sci. Technol. **26**, 014037 (2011). [doi:10.1088/0268-1242/26/1/014037]
205. “Advances in electronic structure methods for defects and impurities in solids”, C. G. Van de Walle and A. Janotti, Phys. Status Solidi B **248**, 19 (2011). [doi: 10.1002/pssb.201046290]
206. “Tin dioxide from first principles: Quasiparticle electronic states and optical properties”, A. Schleife, J. B. Varley, F. Fuchs, C. Rödl, F. Bechstedt, P. Rinke, A. Janotti, and C. G. Van de Walle, Phys. Rev. B **83**, 035116 (2011); **87**, 239901(E) (2013). [doi: 10.1103/PhysRevB.83.035116]
207. “Native defects in Al₂O₃ and their impact on III-V/ Al₂O₃ metal-oxide-semiconductor-based devices”, J. R. Weber, A. Janotti, and C. G. Van de Walle, J. Appl. Phys. **109**, 033715 (2011). [doi: 10.1063/1.3544310]
208. “Hybrid functional investigations of band gaps and band alignments for AlN, GaN, InN, and InGaN”, P. G. Moses, M. Miao, Q. Yan, and C. G. Van de Walle, J. Chem. Phys. **134**, 084703 (2011). [doi: [10.1063/1.3548872](https://doi.org/10.1063/1.3548872)]

209. "Indirect Auger recombination as a cause of efficiency droop in nitride light-emitting diodes", E. Kioupakis, P. Rinke, K. T. Delaney, and C. G. Van de Walle, *Appl. Phys. Lett.* **98**, 161107 (2011). [doi: [10.1063/1.3570656](https://doi.org/10.1063/1.3570656)]
210. "Mechanism of visible-light photocatalysis in nitrogen-doped TiO₂", J. B. Varley, A. Janotti, and C. G. Van de Walle, *Adv. Mater.* **23**, 2343 (2011). [doi: [10.1002/adma.201003603](https://doi.org/10.1002/adma.201003603)]
211. "The particle-size dependence of the activation energy for decomposition of lithium amide", K. Hoang, A. Janotti, and C. G. Van de Walle, *Angew. Chem. Int. Ed.* **50**, 10170 (2011). [doi: [10.1002/anie.201100810](https://doi.org/10.1002/anie.201100810)]
212. "Defects in SiC for quantum computing", J. R. Weber, W. F. Koehl, J. B. Varley, A. Janotti, B. B. Buckley, C. G. Van de Walle, and D. D. Awschalom, *J. Appl. Phys.* **109**, 102417 (2011). [doi: [10.1063/1.3578264](https://doi.org/10.1063/1.3578264)]
213. "The role of oxygen-related defects and hydrogen impurities in HfO₂ and ZrO₂", J. L. Lyons, A. Janotti, and C. G. Van de Walle, *Microel. Eng.* **88**, 1452 (2011). [doi: [10.1016/j.mee.2011.03.099](https://doi.org/10.1016/j.mee.2011.03.099)]
214. "Insulating state of ultrathin epitaxial LaNiO₃ thin films detected by hard x-ray photoemission", A. X. Gray, A. Janotti, J. Son, J. M. LeBeau, S. Ueda, Y. Yamashita, K. Kobayashi, A. M. Kaiser, R. Sutarto, H. Wadati, G. A. Sawatzky, C. G. Van de Walle, S. Stemmer, and C. S. Fadley, *Phys. Rev. B* **84**, 075104 (2011). [doi: [10.1103/PhysRevB.84.075104](https://doi.org/10.1103/PhysRevB.84.075104)]
215. "High optical polarization ratio from semipolar (20-2-1) blue-green InGaN/GaN light-emitting diodes", Y. Zhao, S. Tanaka, Q. Yan, C.-Y. Huang, R. B. Chung, C.-C. Pan, K. Fujito, D. Feezell, C. G. Van de Walle, J. S. Speck, S. P. DenBaars, and S. Nakamura, *Appl. Phys. Lett.* **99**, 051109 (2011). [doi: [10.1063/1.3619826](https://doi.org/10.1063/1.3619826)] (Publisher's note: publication error corrected, *Appl. Phys. Lett.* **99**, 229902 (2011). [doi: [10.1063/1.3665683](https://doi.org/10.1063/1.3665683)])
216. "Hydrogenated cation vacancies in semiconducting oxides", J. B. Varley, H. Peelaers, A. Janotti and C. G. Van de Walle, *J. Phys. Condens. Matter* **23**, 334212 (2011). [doi: [10.1088/0953-8984/23/33/334212](https://doi.org/10.1088/0953-8984/23/33/334212)]
217. "LDA+*U* and hybrid functional calculations for defects in ZnO, SnO₂, and TiO₂", A. Janotti and C. G. Van de Walle, *Phys. Status Solidi B* **248**, 799 (2011). [doi: [10.1002/pssb.201046384](https://doi.org/10.1002/pssb.201046384)]
218. "Electrostatic interactions between charged defects in supercells", C. Freysoldt, J. Neugebauer, and C. G. Van de Walle, *Phys. Status Solidi B* **248**, 1067 (2011). [doi: [10.1002/pssb.201046289](https://doi.org/10.1002/pssb.201046289)]
219. "Influence of Mg-doped barriers on semipolar (20-2-1) multiple-quantum-well green light-emitting diodes", C.-Y. Huang, Q. Yan, Y. Zhao, K. Fujito, D. Feezell, C. G. Van de Walle, J. S. Speck, S. P. DenBaars, and S. Nakamura, *Appl. Phys. Lett.* **99**, 141114 (2011). [doi: [10.1063/1.3647560](https://doi.org/10.1063/1.3647560)]

220. “Stability and mobility of native point defects in AlH₃”, L. Ismer, A. Janotti, and C. G. Van de Walle, *J. Alloys Compd.* **509S**, S658 (2011). [doi:10.1016/j.jallcom.2010.10.014]
221. “Experimental electronic structure of In₂O₃ and Ga₂O₃”, C. Janowitz, V. Scherer, M. Mohamed, A. Krapf, H. Dwelk, R. Manzke, Z. Galazka, R. Uecker, K. Irscher, R. Fornari, M. Michling, D. Schmeißer, J. R Weber, J. B Varley, and C. G Van de Walle, *New J. Phys.* **13**, 085014 (2011). [doi:10.1088/1367-2630/13/8/085014]
222. “Strain effects on the electronic structure of SrTiO₃: Toward high electron mobilities”, A. Janotti, D. Steiauf, and C. G. Van de Walle, *Phys. Rev. B* **84**, 201304(R) (2011). [doi: 10.1103/PhysRevB.84.201304]
223. “Decomposition mechanism and the effects of metal additives on the kinetics of lithium alanate”, K. Hoang, A. Janotti, and C. G. Van de Walle, *Phys. Chem. Chem. Phys.* **14**, 2840 (2012). [doi: 10.1039/c2cp23253g]
224. “Mechanism for the decomposition of lithium borohydride”, K. Hoang and C. G. Van de Walle, *Int. J. Hydrogen Energy* **37**, 5825 (2012). [doi: 10.1016/j.ijhydene.2012.01.002]
225. “Electrostatic carrier doping of GdTiO₃/SrTiO₃ interfaces”, P. Moetakef, T. A. Cain, D. G. Ouellette, J. Y. Zhang, D. O. Klenov, A. Janotti, C. G. Van de Walle, S. Rajan, S. J. Allen, and S. Stemmer, *Appl. Phys. Lett.* **99**, 232116 (2011). [doi: 10.1063/1.3669402]
226. “Hybrid functional calculations of native point defects in InN”, A. Janotti, J. L. Lyons and C. G. Van de Walle, *Phys. Stat. Sol. A* **209**, 65 (2012). [doi: 10.1002/pssa.201100216]
227. “Mechanisms for the decomposition and dehydrogenation of Li amide/imide”, K. Hoang, A. Janotti, and C. G. Van de Walle, *Phys. Rev. B* **85**, 064115 (2012). [doi: 10.1103/PhysRevB.85.064115]
228. “Fundamental limits on optical transparency of transparent conducting oxides: Free-carrier absorption in SnO₂”, H. Peelaers, E. Kioupakis, and C. G. Van de Walle, *Appl. Phys. Lett.* **100**, 011914 (2012). [doi: [10.1063/1.3671162](https://doi.org/10.1063/1.3671162)]
229. “Role of self-trapping in luminescence and *p*-type conductivity of wide-band-gap oxides”, J. Varley, A. Janotti, C. Franchini, and C. G. Van de Walle, *Phys. Rev. B* **85**, 081109 (2012). [doi: [10.1103/PhysRevB.85.081109](https://doi.org/10.1103/PhysRevB.85.081109)]
230. “First-Principles Optical Spectra for F Centers in MgO”, P. Rinke, A. Schleife, E. Kioupakis, A. Janotti, C. Rödl, F. Bechstedt, M. Scheffler, and C. G. Van de Walle, *Phys. Rev. Lett.* **108**, 126404 (2012). [doi: [10.1103/PhysRevLett.108.126404](https://doi.org/10.1103/PhysRevLett.108.126404)]
231. “Role of nitrogen vacancies in the luminescence of Mg-doped GaN”, Q. Yan, A. Janotti, M. Scheffler, and C. G. Van de Walle, *Appl. Phys. Lett.* **100**, 142110 (2012). [doi: 10.1063/1.3699009]

232. “Confinement effects on valence-subband character and polarization anisotropy in (11-22) semipolar InGaN/GaN quantum wells”, C. Roberts, Q. Yan, M. S. Miao, and C. G. Van de Walle, *J. Appl. Phys.* **111**, 073113 (2012). [doi: 10.1063/1.3702798]
233. “Indium incorporation and emission properties of nonpolar and semipolar InGaN quantum wells”, Y. Zhao, Q. Yan, C.-Y. Huang, S.-C. Huang, P. S. Hsu, S. Tanaka, C.-C. Pan, Y. Kawaguchi, K. Fujito, C. G. Van de Walle, J. S. Speck, S. P. DenBaars, S. Nakamura, and D. Feezell, *Appl. Phys. Lett.* **100**, 201108 (2012). [doi: 10.1063/1.4719100]
234. “Shallow versus deep nature of Mg acceptors in nitride semiconductors”, J. L. Lyons, A. Janotti, and C. G. Van de Walle, *Phys. Rev. Lett.* **108**, 156403 (2012). [doi: [10.1103/PhysRevLett.108.156403](https://doi.org/10.1103/PhysRevLett.108.156403)]
235. “Influence of polarity on carrier transport in semipolar (20-2-1) and (20-21) multiple-quantum-well light-emitting diodes”, Y. Kawaguchi, C.-Y. Huang, Y.-R. Wu, Q. Yan, C.-C. Pan, Y. Zhao, S. Tanaka, K. Fujito, D. Feezell, C. G. Van de Walle, S. P. DenBaars, and S. Nakamura, *Appl. Phys. Lett.* **100**, 231110 (2012). [doi: 10.1063/1.4726106]
236. “Measurement and Control of Single Nitrogen-Vacancy Center Spins above 600 K”, D. M. Toyli, D. J. Christle, A. Alkauskas, B. B. Buckley, C. G. Van de Walle, and D. D. Awschalom, *Phys. Rev. X* **2**, 031001 (2012). [doi: 10.1103/PhysRevX.2.031001]
237. “Dehydrogenation of AlH₃ via the Vacancy Clustering Mechanism”, L. Ismer, A. Janotti, and C. G. Van de Walle, *J. Phys. Chem. C* **116**, 12995 (2012). [doi: 10.1021/jp211164g]
238. “Effects of doping on the lattice parameter of SrTiO₃”, A. Janotti, B. Jalan, S. Stemmer, and C. G. Van de Walle, *Appl. Phys. Lett.* **100**, 262104 (2012). [doi: 10.1063/1.4730998]
239. “Phonon-assisted optical absorption in silicon from first principles”, J. Noffsinger, E. Kioupakis, C. G. Van de Walle, S. G. Louie, and M. L. Cohen, *Phys. Rev. Lett.* **108**, 167402 (2012). [doi: [10.1103/PhysRevLett.108.167402](https://doi.org/10.1103/PhysRevLett.108.167402)]
240. “Strain effects and band parameters in MgO, ZnO, and CdO”, Q. Yan, P. Rinke, M. Winkelkemper, A. Qteish, D. Bimberg, M. Scheffler, and C. G. Van de Walle, *Appl. Phys. Lett.* **101**, 152105 (2012). [doi: 10.1063/1.4759107]
241. “Polarization-driven topological insulator transition in a GaN/InN/GaN quantum well”, M. S. Miao, Q. Yan, C. G. Van de Walle, W. K. Lou, L. L. Li, and K. Chang, *Phys. Rev. Lett.* **109**, 186803 (2012). [doi: [10.1103/PhysRevLett.109.186803](https://doi.org/10.1103/PhysRevLett.109.186803)]
242. “Interplay of polarization fields and Auger recombination in the efficiency droop of nitride light-emitting diodes”, E. Kioupakis, Q. Yan, and C. G. Van de Walle, *Appl. Phys. Lett.* **101**, 231107 (2012). [doi: [10.1063/1.4769374](https://doi.org/10.1063/1.4769374)]
243. “Effects of strain on band structure and effective masses in MoS₂”, H. Peelaers and C. G. Van de Walle, *Phys. Rev. B* **86**, 241401(R) (2012). [doi:10.1103/PhysRevB.86.241401]

244. “First-principles calculations of luminescence spectrum line shapes for defects in semiconductors: the example of GaN and ZnO”, A. Alkauskas, J. L. Lyons, D. Steiauf, and C. G. Van de Walle, *Phys. Rev. Lett.* **109**, 267401 (2012). [doi: [10.1103/PhysRevLett.109.267401](https://doi.org/10.1103/PhysRevLett.109.267401)]
245. “Controlling the density of the two-dimensional electron gas at the SrTiO₃/LaAlO₃ interface”, A. Janotti, L. Bjaalie, L. Gordon, and C. G. Van de Walle, *Phys. Rev. B* **86**, 241108(R) (2012). [doi: [10.1103/PhysRevB.86.241108](https://doi.org/10.1103/PhysRevB.86.241108)]
246. “Electrically active Er doping in InAs, In_{0.53}Ga_{0.47}As, and GaAs”, P. G. Burke, L. Ismer, H. Lu, E. Frantz, A. Janotti, C. G. Van de Walle, J. E. Bowers, and A. C. Gossard, *Appl. Phys. Lett.* **101**, 232103 (2012). [doi: [10.1063/1.4769248](https://doi.org/10.1063/1.4769248)]
247. “Optical polarization characteristics of semipolar (30-31) and (30-3-1) InGaN/GaN light-emitting diodes”, Y. Zhao, Q. Yan, D. Feezell, K. Fujito, C. G. Van de Walle, J. S. Speck, S. P. DenBaars, and S. Nakamura, *Optics Exp.* **21**, A53 (2013). [doi: [10.1364/OE.21.000A53](https://doi.org/10.1364/OE.21.000A53)]
248. “Native point defects and dangling bonds in α -Al₂O₃”, M. Choi, A. Janotti, and C. G. Van de Walle, *J. Appl. Phys.* **113**, 044501 (2013). [doi: [10.1063/1.4784114](https://doi.org/10.1063/1.4784114)]
249. “Effect of transition-metal additives on hydrogen desorption kinetics of MgH₂”, A. Roy, A. Janotti, and C. G. Van de Walle, *Appl. Phys. Lett.* **102**, 033902 (2013). [doi: [10.1063/1.4788746](https://doi.org/10.1063/1.4788746)]
250. “Enhanced optical absorption due to symmetry breaking in TiO_{2(1-x)}S_{2x} alloys”, A. Schleife, P. Rinke, F. Bechstedt, and C. G. Van de Walle, *J. Phys. Chem. C* **117**, 4189 (2013). [doi: [10.1021/jp3106937](https://doi.org/10.1021/jp3106937)]
251. “Dangling bonds and vacancies in germanium”, J. Weber, A. Janotti, and C. G. Van de Walle, *Phys. Rev. B* **87**, 035203 (2013). [doi: [10.1103/PhysRevB.87.035203](https://doi.org/10.1103/PhysRevB.87.035203)]
252. “Structural origins of the properties of rare earth nickelate superlattices”, J. Hwang, J. Son, J. Y. Zhang, A. Janotti, C. G. Van de Walle, and S. Stemmer, *Phys. Rev. B* **87**, 060101 (2013). [doi: [10.1103/PhysRevB.87.060101](https://doi.org/10.1103/PhysRevB.87.060101)]
253. “Electronic structure of a single-layer InN quantum well in a GaN matrix”, M. S. Miao, Q. M. Yan, and C. G. Van de Walle, *Appl. Phys. Lett.* **102**, 102103 (2013). [doi: [10.1063/1.4794986](https://doi.org/10.1063/1.4794986)]
254. “Dual behavior of excess electrons in rutile TiO₂”, A. Janotti, C. Franchini, J. B. Varley, G. Kresse, and C. G. Van de Walle, *Phys. Status Solidi RRL* **7**, 199 (2013). [doi: [10.1002/pssr.201206464](https://doi.org/10.1002/pssr.201206464)]
255. “Impact of carbon and nitrogen impurities in high- κ dielectrics on metal-oxide-semiconductor-based devices”, M. Choi, J. L. Lyons, A. Janotti, and C. G. Van de Walle, *Appl. Phys. Lett.* **102**, 142902 (2013). [doi: [10.1063/1.4801497](https://doi.org/10.1063/1.4801497)]

256. “Band offsets in complex-oxide thin films and heterostructures of SrTiO₃/LaNiO₃ and SrTiO₃/GdTiO₃ by soft and hard X-ray photoelectron spectroscopy”, G. Conti, A. M. Kaiser, A. X. Gray, S. Nemšák, G. K. Palsson, J. Son, P. Moetakef, A. Janotti, L. Bjaalie, C. S. Conlon, D. Eiteneer, A. A. Greer, A. Keqi, A. Rattanachata, A. Y. Saw, A. Bostwick, W. C. Stolte, A. Gloskovskii, W. Drube, S. Ueda, M. Kobata, K. Kobayashi, C. G. Van de Walle, S. Stemmer, C. M. Schneider, and C. S. Fadley, *J. Appl. Phys.* **113**, 143704 (2013). [doi: 10.1063/1.4795612]
257. “Effects of strain on the electron effective mass in GaN and AlN”, C. E. Dreyer, A. Janotti, and C. G. Van de Walle, *Appl. Phys. Lett.* **102**, 142105 (2013). [doi: 10.1063/1.4801520]
258. “Impact of native defects in high-k dielectric oxides on GaN/oxide metal–oxide–semiconductor devices”, M. Choi, J. L. Lyons, A. Janotti, and C. G. Van de Walle, *Phys. Status Solidi B* **250**, 787 (2013). [doi: 10.1002/pssb.201200628]
259. “Defects at Ge/oxide and III-V/oxide interfaces”, C. G. Van de Walle, M. Choi, J. R. Weber, J. L. Lyons, and A. Janotti, *Microelectron. Eng.* **109**, 211 (2013). [doi: 10.1016/j.mee.2013.03.151]
260. “Impact of group-II acceptors on the electrical and optical properties of GaN”, J. L. Lyons, A. Janotti, and C. G. Van de Walle, *Jpn. J. Appl. Phys.* **52**, 08JJ04 (2013). [doi: [10.7567/JJAP.52.08JJ04](https://doi.org/10.7567/JJAP.52.08JJ04)]
261. “Polarization effects due to thickness fluctuations in nonpolar InGaN/GaN quantum wells”, O. Marquardt, T. Hickel, J. Neugebauer, and C. G. Van de Walle, *Appl. Phys. Lett.* **103**, 073115 (2013). [doi: 10.1063/1.4818752]
262. “Ambipolar doping in SnO”, J. B. Varley, A. Schleife, A. Janotti, and C. G. Van de Walle, *Appl. Phys. Lett.* **103** (2013). [doi: 10.1063/1.4819068]
263. “Quantum computing with defects”, L. Gordon, J. R. Weber, J. B. Varley, A. Janotti, D. D. Awschalom, and C. G. Van de Walle, *MRS Bull.* **38**, 802 (2013). [doi: 10.1557/mrs.2013.206]
264. “LiH as a Li⁺ and H⁻ ion provider”, K. Hoang and C. G. Van de Walle, *Solid State Ionics* **253**, 53 (2013). [doi: 10.1016/j.ssi.2013.08.017]
265. “Temperature and carrier-density dependence of Auger and radiative recombination in nitride optoelectronic devices”, E. Kioupakis, Q. Yan, D. Steiauf, and C. G. Van de Walle, *New J. Phys.* **15**, 125006 (2013). [doi: [10.1088/1367-2630/15/12/125006](https://doi.org/10.1088/1367-2630/15/12/125006)]
266. “Native point defects in LaAlO₃: A hybrid functional study”, M. Choi, A. Janotti, and C. G. Van de Walle, *Phys. Rev. B* **88**, 214117 (2013). [doi: [10.1103/PhysRevB.88.214117](https://doi.org/10.1103/PhysRevB.88.214117)]
267. “Effects of hole localization on limiting *p*-type conductivity in oxide and nitride semiconductors”, J. L. Lyons, A. Janotti, and C. G. Van de Walle, *J. Appl. Phys.* **115**, 012014 (2014). [doi: [10.1063/1.4838075](https://doi.org/10.1063/1.4838075)]

268. “Effects of carbon on the electrical and optical properties of InN, GaN, and AlN”, J. L. Lyons, A. Janotti, and C. G. Van de Walle, *Phys. Rev. B* **89**, 035204 (2014). [doi:[10.1103/PhysRevB.89.035204](https://doi.org/10.1103/PhysRevB.89.035204)]
269. “Band alignments and polarization properties of BN polymorphs”, C. E. Dreyer, J. L. Lyons, A. Janotti, and C. G. Van de Walle, *Appl. Phys. Express* **7**, 031001 (2014). [doi:[10.7567/APEX.7.031001](https://doi.org/10.7567/APEX.7.031001)]; **13**, 019301 (2020) (erratum). [doi: [10.7567/1882-0786/ab5e1c](https://doi.org/10.7567/1882-0786/ab5e1c)]
270. “Absolute surface energies of polar and nonpolar planes of GaN”, C. E. Dreyer, A. Janotti, and C. G. Van de Walle, *Phys. Rev. B* **89**, 081305(R) (2014). [doi: 10.1103/PhysRevB.89.081305]
271. “Oxide interfaces for novel electronic applications”, L. Bjaalie, B. Himmetoglu, L. Weston, A. Janotti and C. G. Van de Walle, *New J. Phys.* **16**, 025005 (2014). [doi: [10.1088/1367-2630/16/2/025005](https://doi.org/10.1088/1367-2630/16/2/025005)]
272. “Hydrogenated vacancies and hidden hydrogen in SrTiO₃”, J. B. Varley, A. Janotti, and C. G. Van de Walle, *Phys. Rev. B* **89**, 075202 (2014). [doi: [10.1103/PhysRevB.89.075202](https://doi.org/10.1103/PhysRevB.89.075202)]
273. “Hybrid functional calculations of DX centers in AlN and GaN”, L. Gordon, J. L. Lyons, A. Janotti and C. G. Van de Walle, *Phys. Rev. B* **89**, 085204 (2014). [doi: 10.1103/PhysRevB.89.085204]
274. “Hydrogen passivation of impurities in Al₂O₃”, M. Choi, A. Janotti, and C. G. Van de Walle, *ACS Appl. Mater. Interfaces* **6**, 4149 (2014). [doi: 10.1021/am4057997]
275. “Elastic Constants and Pressure-Induced Effects in MoS₂”, H. Peelaers and C. G. Van de Walle, *J. Phys. Chem. C* **118**, 12073 (2014). [doi:10.1021/jp503683h]
276. “Band alignment at band-insulator/Mott-insulator interfaces”, A. Janotti, L. Bjaalie, B. Himmetoglu, and C. G. Van de Walle, *Phys. Status Solidi RRL* **8**, 577 (2014). [doi: 10.1002/pssr.201409088]
277. “High-voltage field effect transistors with wide-bandgap β -Ga₂O₃ nanomembranes”, W. S. Hwang, A. Verma, H. Peelaers, V. Protasenko, S. Rouvimov, H. G. Xing, A. Seabaugh, W. Haensch, C. Van de Walle, Z. Galazka, M. Albrecht, R. Fornari, and D. Jena, *Appl. Phys. Lett.* **104**, 203111 (2014). [doi:10.1063/1.4879800]
278. “Hybrid functional calculations of point defects and hydrogen in SrZrO₃”, L. Weston, A. Janotti, X. Y. Cui, C. Stampfl, and C. G. Van de Walle, *Phys. Rev. B* **89**, 184109 (2014). [doi: : 10.1103/PhysRevB.89.184109]
279. “First-principles study of van der Waals interactions in MoS₂ and MoO₃”, H. Peelaers and C.G. Van de Walle, *J. Phys. Condens. Matter* **26**, 305502 (2014). [doi:10.1088/0953-8984/26/30/305502]

280. “First-principles theory of the luminescence lineshape for the triplet transition in diamond NV centres”, A. Alkauskas, B. B. Buckley, D. D. Awschalom, and C. G. Van de Walle, *New J. Phys.* **16**, 073026 (2014). [doi:[10.1088/1367-2630/16/7/073026](https://doi.org/10.1088/1367-2630/16/7/073026)]
281. “First-principles theory of nonradiative carrier capture via multiphonon emission”, A. Alkauskas, Q. Yan, and C. G. Van de Walle, *Phys. Rev. B* **90**, 075202 (2014). [doi:[10.1103/PhysRevB.90.075202](https://doi.org/10.1103/PhysRevB.90.075202)]
282. “Vacancies and small polarons in SrTiO₃”, A. Janotti, M. Choi, J. B. Varley, and C. G. Van de Walle, *Phys. Rev. B* **90**, 085202 (2014). [doi:[10.1103/PhysRevB.90.085202](https://doi.org/10.1103/PhysRevB.90.085202)]
283. “Direct View at Excess Electrons in TiO₂ Rutile and Anatase”, M. Setvin, C. Franchini, X. Hao, M. Schmid, A. Janotti, M. Kaltak, C. G. Van de Walle, G. Kresse, and U. Diebold, *Phys. Rev. Lett.* **113**, 086402 (2014). [doi: [10.1103/PhysRevLett.113.086402](https://doi.org/10.1103/PhysRevLett.113.086402)]
284. “Auger Recombination in GaAs from First Principles”, D. Steiauf, E. Kioupakis, and C. G. Van de Walle, *ACS Photonics* **1**, 643 (2014). [doi:[10.1021/ph500119q](https://doi.org/10.1021/ph500119q)]
285. “Effects of In profile on simulations of InGaN/GaN multi-quantum-well light-emitting diode”, P. M. McBride, Q. Yan, and C. G. Van de Walle, *Appl. Phys. Lett.* **105**, 083507 (2014). [doi:[10.1063/1.4894464](https://doi.org/10.1063/1.4894464)]
286. “First-principles study of vacancy-assisted impurity diffusion in ZnO”, D. Steiauf, J. L. Lyons, A. Janotti, and C. G. Van de Walle, *APL Materials* **2**, 096101 (2014). [doi:[10.1063/1.4894195](https://doi.org/10.1063/1.4894195)]
287. “First-principles study of high-field-related electronic behavior of group-III nitrides”, Q. Yan, E. Kioupakis, D. Jena, and C. G. Van de Walle, *Phys. Rev. B* **90**, 121201(R) (2014). [doi: [10.1103/PhysRevB.90.121201](https://doi.org/10.1103/PhysRevB.90.121201)]
288. “Origins of optical absorption and emission lines in AlN”, Q. Yan, A. Janotti, M. Scheffler, and C. G. Van de Walle, *Appl. Phys. Lett.* **105**, 111104 (2014). [doi: [10.1063/1.4895786](https://doi.org/10.1063/1.4895786)]
289. “Effects of strain on the band structure of group-III nitrides”, Q. Yan, P. Rinke, A. Janotti, M. Scheffler, and C. G. Van de Walle, *Phys. Rev. B* **90**, 125118 (2014). [doi: [10.1103/PhysRevB.90.125118](https://doi.org/10.1103/PhysRevB.90.125118)]
290. “Interband and polaronic excitations in YTiO₃ from first principles”, B. Himmetoglu, A. Janotti, L. Bjaalie, and C. G. Van de Walle, *Phys. Rev. B* **90**, 161102(R) (2014). [doi:[10.1103/PhysRevB.90.161102](https://doi.org/10.1103/PhysRevB.90.161102)]
291. “Carbon-induced trapping levels in oxide dielectrics”, H. D. Taylor, J. L. Lyons, M. Choi, A. Janotti, and C. G. Van de Walle, *J. Vac. Sci. Tech. A* **33**, 01A120 (2015). [doi: [10.1116/1.4901234](https://doi.org/10.1116/1.4901234)]
292. “Turning SrTiO₃ into a Mott insulator”, L. Bjaalie, A. Janotti, B. Himmetoglu, and C. G. Van de Walle, *Phys. Rev. B* **90**, 195117 (2014). [doi: [10.1103/PhysRevB.90.195117](https://doi.org/10.1103/PhysRevB.90.195117)]

293. “The role of native defects in the transport of charge and mass and the decomposition of $\text{Li}_4\text{BN}_3\text{H}_{10}$ ”, K. Hoang, A. Janotti, and C. G. Van de Walle, *Phys. Chem. Chem. Phys.* **16**, 25314 (2014). [doi: : 10.1039/c4cp03677h]
294. “Ferroelastic switching of doped zirconia: Modeling and understanding from first principles”, C. Carbogno, C. G. Levi, C. G. Van de Walle, and M. Scheffler, *Phys. Rev. B* **90**, 144109 (2014). [doi: 10.1103/PhysRevB.90.144109]
295. “Nature and evolution of the band-edge states in MoS_2 : From monolayer to bulk”, J. E. Padilha, H. Peelaers, A. Janotti, and C. G. Van de Walle, *Phys. Rev. B* **90**, 205420 (2014). [doi: 10.1103/PhysRevB.90.205420]
296. “Carbon as a shallow donor in transparent conducting oxides”, J. L. Lyons, D. Steiauf, A. Janotti, and C. G. Van de Walle, *Phys. Rev. Appl.* **2**, 064005 (2014). [doi: 10.1103/PhysRevApplied.2.064005]
297. “First-principles study of the mobility of SrTiO_3 ”, B. Himmetoglu, A. Janotti, H. Peelaers, A. Alkauskas, and C. G. Van de Walle, *Phys. Rev. B* **90**, 241204(R) (2014). [doi:10.1103/PhysRevB.90.241204]
298. “Structure and energetics of LaAlO_3 (001) surfaces”, K. Krishnaswamy, C. E. Dreyer, A. Janotti, and C. G. Van de Walle, *Phys. Rev. B* **90**, 235436 (2014). [doi:10.1103/PhysRevB.90.235436]
299. “Hydrogen bonds in Al_2O_3 as dissipative two-level systems in superconducting qubits”, L. Gordon, H. Abu Farsakh, A. Janotti, and C. G. Van de Walle, *Sci. Rep.* **4**, 7590 (2014). [doi: [10.1038/srep07590](https://doi.org/10.1038/srep07590)]
300. “Nitride-based high-electron-mobility transistor with single-layer InN for mobility-enhanced channel”, M. S. Miao and C. G. Van de Walle, *Appl. Phys. Express* **8**, 024302 (2015). [doi: 10.7567/APEX.8.024302]
301. “Limitations to the room temperature mobility of two- and three-dimensional electron liquids in SrTiO_3 ”, E. Mikheev, B. Himmetoglu, A. P. Kajdos, P. Moetakef, T. A. Cain, C. G. Van de Walle, and S. Stemmer, *Appl. Phys. Lett.* **106**, 062102 (2015). [doi: 10.1063/1.4907888]
302. “Brillouin zone and band structure of $\beta\text{-Ga}_2\text{O}_3$ ”, H. Peelaers and C.G. Van de Walle, *Phys. Status Solidi B* **252**, 828 (2015). [doi: [10.1002/pssb.201451551](https://doi.org/10.1002/pssb.201451551)]
303. “First-principles theory of acceptors in nitride semiconductors”, J. L. Lyons, A. Alkauskas, A. Janotti, and C. G. Van de Walle, *Phys. Stat. Sol. B* **252**, 900 (2015). [doi: [10.1002/pssb.201552062](https://doi.org/10.1002/pssb.201552062)]
304. “Small hole polarons in rare-earth titanates”, L. Bjaalie, D. G. Ouellette, P. Moetakef, T. A. Cain, A. Janotti, B. Himmetoglu, S. J. Allen, S. Stemmer, and C. G. Van de Walle, *Appl. Phys. Lett.* **106**, 232103 (2015). [doi: [10.1063/1.4922316](https://doi.org/10.1063/1.4922316)]

305. “Defects as qubits in 3C- and 4H-SiC”, L. Gordon, A. Janotti, and C. G. Van de Walle, Phys. Rev. B **92**, 045208 (2015). [doi: [10.1103/PhysRevB.92.045208](https://doi.org/10.1103/PhysRevB.92.045208)]
306. “Brittle fracture toughnesses of GaN and AlN from first-principles surface-energy calculations”, C. E. Dreyer, A. Janotti, and C. G. Van de Walle, Appl. Phys. Lett. **106**, 212103 (2015). [doi: [10.1063/1.4921855](https://doi.org/10.1063/1.4921855)]
307. “Determination of the Mott-Hubbard gap in GdTiO₃”, L. Bjaalie, A. Verma, B. Himmetoglu, A. Janotti, S. Raghavan, V. Protasenko, E. H. Steenbergen, D. Jena, S. Stemmer, and C. G. Van de Walle, Phys. Rev. B **92**, 085111 (2015). [doi: [10.1103/PhysRevB.92.085111](https://doi.org/10.1103/PhysRevB.92.085111)]
308. “First-principles calculations of indirect Auger recombination in nitride semiconductors”, E. Kioupakis, D. Steiauf, P. Rinke, K. T. Delaney, and C. G. Van de Walle, Phys. Rev. B **92**, 035207 (2015). [doi: [10.1103/PhysRevB.92.035207](https://doi.org/10.1103/PhysRevB.92.035207)]
309. “Sulfur doping of AlN and AlGaN for improved *n*-type conductivity”, L. Gordon, J. B. Varley, J. L. Lyons, A. Janotti, and C. G. Van de Walle, Phys. Status Solidi RRL **9**, 462 (2015). [doi: [10.1002/pssr.201510165](https://doi.org/10.1002/pssr.201510165)]
310. “(In_xGa_{1-x})₂O₃ alloys for transparent electronics”, H. Peelaers, D. Steiauf, J. B. Varley, A. Janotti, and C. G. Van de Walle, Phys. Rev. B **92**, 085206 (2015). [doi: [10.1103/PhysRevB.92.085206](https://doi.org/10.1103/PhysRevB.92.085206)]
311. “First-principles study of surface charging in LaAlO₃/SrTiO₃ heterostructures”, K. Krishnaswamy, C. E. Dreyer, A. Janotti, and C. G. Van de Walle, Phys. Rev. B **92**, 085420 (2015). [doi: [10.1103/PhysRevB.92.085420](https://doi.org/10.1103/PhysRevB.92.085420)]
312. “Structural and electronic properties of SrZrO₃ and Sr(Ti,Zr)O₃ alloys”, L. Weston, A. Janotti, X. Y. Cui, B. Himmetoglu, C. Stampfl, and C. G. Van de Walle, Phys. Rev. B **92**, 085201 (2015). [doi: [10.1103/PhysRevB.92.085201](https://doi.org/10.1103/PhysRevB.92.085201)]
313. “High optical power and low efficiency droop blue light-emitting diodes using compositionally step-graded InGa_N barrier”, C.-C. Pan, Q. Yan, H. Fu, Y. Zhao, Y. R. Wu, C. Van de Walle, S. Nakamura, and S. P. DenBaars, Electron. Lett. **51**, 1187 (2015). [doi: [10.1049/el.2015.1647](https://doi.org/10.1049/el.2015.1647)]
314. “Impact of electric-field dependent dielectric constants on two-dimensional electron gases in complex oxides”, H. Peelaers, K. Krishnaswamy, L. Gordon, D. Steiauf, A. Sarwe, A. Janotti, and C. G. Van de Walle, Appl. Phys. Lett. **107**, 183505 (2015). [doi: [10.1063/1.4935222](https://doi.org/10.1063/1.4935222)]
315. “Tuning bad metal and non-Fermi liquid behavior in a Mott material: Rare-earth nickelate thin films”, E. Mikheev, A. J. Hauser, B. Himmetoglu, N. E. Moreno, A. Janotti, C. G. Van de Walle, and S. Stemmer, Sci. Adv. **1**, e1500797 (2015). [doi: [10.1126/sciadv.1500797](https://doi.org/10.1126/sciadv.1500797)]

316. "Free-carrier absorption in transparent conducting oxides: Phonon and impurity scattering in SnO₂", H. Peelaers, E. Kioupakis, and C.G. Van de Walle, *Phys. Rev. B* **92**, 235201 (2015). [doi: 10.1103/PhysRevB.92.235201]
317. "Exciton-dominated Dielectric Function of Atomically Thin MoS₂ Films", Y. Yu, Y. Yu, Y. Cai, W. Li, A. Gurarslan, H. Peelaers, D. E. Aspnes, C. G. Van de Walle, N. V. Nguyen, Y.-W. Zhang, and L. Cao, *Sci. Rep.* **5**, 16996 (2015). [doi: 10.1038/srep16996]
318. "Observation by resonant angle-resolved photoemission of a critical thickness for 2-dimensional electron gas formation in SrTiO₃ embedded in GdTiO₃", S. Nemšák, G. Conti, G. K. Palsson, C. Conlon, S. Cho, J. E. Rault, J. Avila, M.-C. Asensio, C. A. Jackson, P. Moetakef, A. Janotti, L. Bjaalie, B. Himmetoglu, C. G. Van de Walle, L. Balents, C. M. Schneider, S. Stemmer and C. S. Fadley, *Appl. Phys. Lett.* **107**, 231602 (2015). [doi: 10.1063/1.4936936]
319. "Effects of biaxial stress and layer thickness on octahedral tilts in LaNiO₃", P. M. McBride, A. Janotti, C. E. Dreyer, B. Himmetoglu, and C. G. Van de Walle, *Appl. Phys. Lett.* **107**, 261901 (2015). [doi: 10.1063/1.4939002]
320. "Small polarons and point defects in barium cerate", M. Swift, A. Janotti, and C. G. Van de Walle, *Phys. Rev. B* **92**, 214114 (2015). [doi: 10.1103/PhysRevB.92.214114]
321. "Identification of microscopic hole-trapping mechanisms in nitride semiconductors," J. L. Lyons, K. Krishnaswamy, L. Gordon, A. Janotti, and C. G. Van de Walle, *IEEE Electron Device Lett.* **37**, 154 (2016). [doi: [10.1109/LED.2015.2509068](https://doi.org/10.1109/LED.2015.2509068)]
322. "Surprising stability of neutral interstitial hydrogen in diamond and cubic BN", J. L. Lyons and C. G. Van de Walle, *J. Phys.: Condens. Matter* **28**, 06LT01 (2016). [doi:10.1088/0953-8984/28/6/06LT01]
323. "BaSnO₃ as a channel material in perovskite oxide heterostructures", K. Krishnaswamy, L. Bjaalie, B. Himmetoglu, A. Janotti, L. Gordon, and C. G. Van de Walle, *Appl. Phys. Lett.* **108**, 083501 (2016). [doi: [10.1063/1.4942366](https://doi.org/10.1063/1.4942366)]
324. "Point-defect kinetics in α - and γ -MgH₂", J. M. Sander, L. Ismer, and C. G. Van de Walle, *Int. J. Hydrogen Energy* **41**, 5688 (2016). [doi: [10.1016/j.ijhydene.2016.01.156](https://doi.org/10.1016/j.ijhydene.2016.01.156)]
325. "Point defects, impurities, and small hole polarons in GdTiO₃", L. Bjaalie, A. Janotti, K. Krishnaswamy, and C. G. Van de Walle, *Phys. Rev. B* **93**, 115316 (2016). [doi: [10.1103/PhysRevB.93.115316](https://doi.org/10.1103/PhysRevB.93.115316)]
326. "Gallium vacancy complexes as a cause of Shockley-Read-Hall recombination in III-nitride light emitters", C. E. Dreyer, A. Alkauskas, J. L. Lyons, J. S. Speck, and C. G. Van de Walle, *Appl. Phys. Lett.* **108**, 141101 (2016). [doi: [10.1063/1.4942674](https://doi.org/10.1063/1.4942674)]
327. "Defects in AlN as candidates for solid-state qubits", J. B. Varley, A. Janotti, and C. G. Van de Walle, *Phys. Rev. B* **93**, 161201 (2016). [doi: [10.1103/PhysRevB.93.161201](https://doi.org/10.1103/PhysRevB.93.161201)]

328. “Donor defects and small polarons on the $\text{TiO}_2(110)$ surface”, P. G. Moses, A. Janotti, C. Franchini, G. Kresse, and C. G. Van de Walle, *J. Appl. Phys.* **119**, 181503 (2016). [doi: [10.1063/1.4948239](https://doi.org/10.1063/1.4948239)]
329. “Tutorial: Defects in semiconductors—Combining experiment and theory”, A. Alkauskas, M. D. McCluskey, and C. G. Van de Walle", *J. Appl. Phys.* **119**, 181101 (2016). [doi: [10.1063/1.4948245](https://doi.org/10.1063/1.4948245)]
330. “Structural investigation of the bilayer iridate $\text{Sr}_3\text{Ir}_2\text{O}_7$ ”, T. Hogan, L. Bjaalie, L. Zhao, C. Belvin, X. Wang, C. G. Van de Walle, D. Hsieh, and S. D. Wilson, *Phys. Rev. B* **93**, 134110 (2016). [doi: [10.1103/PhysRevB.93.134110](https://doi.org/10.1103/PhysRevB.93.134110)]
331. “Electron and chemical reservoir corrections for point-defect formation energies”, C. Freysoldt, B. Lange, J. Neugebauer, Q. Yan, J. L. Lyons, A. Janotti, and C. G. Van de Walle, *Phys. Rev. B* **93**, 165206 (2016). (Editor’s suggestion) [doi: [10.1103/PhysRevB.93.165206](https://doi.org/10.1103/PhysRevB.93.165206)]
332. “Impact of point defects on proton conduction in strontium cerate”, M. Swift and C. G. Van de Walle, *J. Phys. Chem. C* **120**, 9562 (2016). [doi: [10.1021/acs.jpcc.6b00765](https://doi.org/10.1021/acs.jpcc.6b00765)]
333. “Role of excited states in Shockley-Read-Hall recombination in wide-band-gap semiconductors”, A. Alkauskas, C. E. Dreyer, J. L. Lyons, and C. G. Van de Walle, *Phys. Rev. B* **93**, 201304(R) (2016). [doi: [10.1103/PhysRevB.93.201304](https://doi.org/10.1103/PhysRevB.93.201304)]
334. “Energetic, spatial and momentum character of the electronic structure at a buried interface: The two-dimensional electron gas between two metal oxides”, S. Nemšák, G. Conti, A. X. Gray, G. K. Pálsson, C. Conlon, D. Eiteneer, A. Keqi, A. Rattanachata, A. Y. Saw, A. Bostwick, L. Moreschini, E. Rotenberg, V. Strocov, M. Kobayashi, W. Stolte, S. Ueda, K. Kobayashi, A. Gloskovskii, W. Drube, C. Jackson, P. Moetakef, A. Janotti, L. Bjaalie, B. Himmetoglu, C. G. Van de Walle, S. Borek, J. Minar, J. Braun, H. Ebert, L. Plucinski, J. B. Kortright, C. M. Schneider, L. Balents, F. M. F. de Groot, S. Stemmer, and C. S. Fadley, *Phys. Rev. B* **93**, 245103 (2016). [doi: [10.1103/PhysRevB.93.245103](https://doi.org/10.1103/PhysRevB.93.245103)]
335. “Correct implementation of polarization constants in wurtzite materials and impact on III-nitrides”, C. E. Dreyer, A. Janotti, C. G. Van de Walle, and D. Vanderbilt, *Phys. Rev. X* **6**, 021038 (2016). [doi: [10.1103/PhysRevX.6.021038](https://doi.org/10.1103/PhysRevX.6.021038)]
336. “Impact of nitrogen and carbon on defect equilibrium in ZrO_2 ”, H. D. Taylor, J. L. Lyons, C. E. Dreyer, A. Janotti, and C. G. Van de Walle, *Acta Mater.* **117**, 286 (2016). [doi: [10.1016/j.actamat.2016.07.003](https://doi.org/10.1016/j.actamat.2016.07.003)]
337. “Metal versus insulator behavior in ultrathin SrTiO_3 -based heterostructures”, L. Bjaalie, A. Janotti, B. Himmetoglu, and C. G. Van de Walle, *Phys. Rev. B* **94**, 035115 (2016). [doi: [10.1103/PhysRevB.94.035115](https://doi.org/10.1103/PhysRevB.94.035115)]

338. “Depth-Resolved Composition and Electronic Structure of Buried Layers and Interfaces in a $\text{LaNiO}_3/\text{SrTiO}_3$ Superlattice from Soft and Hard X-ray Standing-Wave Angle-Resolved Photoemission”, D. Eiteneer, G. K. Pálsson, S. Nemšák, A. X. Gray, A. M. Kaiser, J. Son, J. LeBeau, G. Conti, A. A. Greer, A. Keqi, A. Rattanachata, A. Y. Saw, A. Bostwick, E. Rotenberg, E. M. Gullikson, S. Ueda, K. Kobayashi, A. Janotti, C. G. Van de Walle, A. Blanca-Romero, R. Pentcheva, C. M. Schneider, S. Stemmer, and C. S. Fadley, *J. Electron Spectrosc.* **211**, 70 (2016). [doi: [10.1016/j.elspec.2016.04.008](https://doi.org/10.1016/j.elspec.2016.04.008)]
339. “Hydrogen intercalation in MoS_2 ”, Z. Zhu, H. Peelaers, and C. G. Van de Walle, *Phys. Rev. B* **94**, 085426 (2016). [doi: [10.1103/PhysRevB.94.085426](https://doi.org/10.1103/PhysRevB.94.085426)]
340. “Role of oxygen vacancies in crystalline WO_3 ”, W. Wang, A. Janotti, and C. G. Van de Walle, *J. Mat Chem. C* **4**, 6641 (2016). [doi: [10.1039/C6TC01643J](https://doi.org/10.1039/C6TC01643J)]
341. “Band alignments between SmTiO_3 , GdTiO_3 , and SrTiO_3 ”, L. Bjaalie, A. Azcatl, S. McDonnell, C. R. Freeze, S. Stemmer, R. M. Wallace, and C. G. Van de Walle, *J. Vac. Sci. Technol. A* **34**, 061102 (2016). [doi: [10.1116/1.4963833](https://doi.org/10.1116/1.4963833)]
342. “Iron as a source of efficient Shockley-Read-Hall recombination in GaN”, D. Wickramaratne, J.-X. Shen, C. E. Dreyer, M. Engel, M. Marsman, G. Kresse, S. Marcinkevičius, A. Alkauskas, C. G. Van de Walle, *Appl. Phys. Lett.* **109**, 162107 (2016). [doi: [10.1063/1.4964831](https://doi.org/10.1063/1.4964831)]
343. “Doping of Ga_2O_3 with transition metals”, H. Peelaers and C. G. Van de Walle, *Phys. Rev. B* **94**, 195203 (2016). [doi: [10.1103/PhysRevB.94.195203](https://doi.org/10.1103/PhysRevB.94.195203)]
344. “Effects of La $5d$ and $4f$ states on the electronic and optical properties of LaAlO_3 ”, J.-X. Shen, A. Schleife, A. Janotti, and C. G. Van de Walle, *Phys. Rev. B* **94**, 205203 (2016). [doi: [10.1103/PhysRevB.94.205203](https://doi.org/10.1103/PhysRevB.94.205203)]
345. “Calcium as a nonradiative recombination center in InGaN”, J.-X. Shen, D. Wickramaratne, C. E. Dreyer, A. Alkauskas, E. Young, J. S. Speck, C. G. Van de Walle, *Appl. Phys. Express* **10**, 021001 (2017). [doi: [10.7567/APEX.10.021001](https://doi.org/10.7567/APEX.10.021001)]
346. “Ab initio study of hydrogenic effective mass impurities in Si nanowires”, H. Peelaers, E. Durgun, B. Partoens, D. I. Bilc, Ph. Ghosez, C. G. Van de Walle, and F. M. Peeters, *J. Phys.: Condens. Matter* **29**, 095303 (2017). [doi: [10.1088/1361-648X/aa5768](https://doi.org/10.1088/1361-648X/aa5768)]
347. “Computationally predicted energies and properties of defects in GaN”, J. L. Lyons and C. G. Van de Walle, *NPJ Comput. Mater.* **3**, 12 (2017). [doi: [10.1038/s41524-017-0014-2](https://doi.org/10.1038/s41524-017-0014-2)]
348. “Controlling n -type doping in MoO_3 ”, H. Peelaers, M. L. Chabinyk, and C. G. Van de Walle, *Chem. Mater.* **29**, 2563 (2017). [doi: [10.1021/acs.chemmater.6b04479](https://doi.org/10.1021/acs.chemmater.6b04479)]
349. “First-principles analysis of electron transport in BaSnO_3 ”, K. Krishnaswamy, B. Himmetoglu, Y. Kang, A. Janotti, and C. G. Van de Walle, *Phys. Rev. B* **95**, 205202 (2017). [doi: [10.1103/PhysRevB.95.205202](https://doi.org/10.1103/PhysRevB.95.205202)]

350. "Identification of yellow luminescence centers in Be-doped GaN through pressure-dependent studies", H. Teisseyre, J. L. Lyons, A. Kaminska, D. Jankowski, D. Jarosz, M. Boćkowski, A. Suchocki and C. G. Van de Walle, *J. Phys. D: Appl. Phys.* **50**, 22LT03 (2017). [doi: [10.1088/1361-6463/aa6e90](https://doi.org/10.1088/1361-6463/aa6e90)]
351. "Acceptor doping in the proton conductor SrZrO₃", L. Weston, A. Janotti, X. Y. Cui, C. Stampfl, and C. G. Van de Walle, *Phys. Chem. Chem. Phys.* **19**, 11485 (2017). [doi: [10.1039/c7cp01471f](https://doi.org/10.1039/c7cp01471f)]
352. "Fundamental limits on the electron mobility of β -Ga₂O₃", Y. Kang, K. Krishnaswamy, H. Peelaers, and C. G. Van de Walle, *J. Phys.: Condens. Matter* **29**, 234001 (2017). [doi: [10.1088/1361-648X/aa6f66](https://doi.org/10.1088/1361-648X/aa6f66)]
353. "Phase transformations upon doping in WO₃", W. Wang, A. Janotti, and C.G. Van de Walle. *J. Chem. Phys.* **146**, 214504 (2017). [doi: [10.1063/1.4984581](https://doi.org/10.1063/1.4984581)]
354. "Conditions for T² resistivity from electron-electron scattering", M. W. Swift and C. G. Van de Walle, *Eur. Phys. J. B* **90**, 151 (2017). [doi: [10.1140/epjb/e2017-80367-1](https://doi.org/10.1140/epjb/e2017-80367-1)]
355. "Electrical compensation mechanism in fluorine-doped SnO₂", Y. Kang and C. G. Van de Walle, *Appl. Phys. Lett.* **111**, 152107 (2017). [doi: [10.1063/1.4999479](https://doi.org/10.1063/1.4999479)]
356. "Growth of coherent BGaN films using BBr₃ gas as a boron source in plasma assisted molecular beam epitaxy", R. C. Cramer, B. Bonaf, J. English, C. E. Dreyer, C. G. Van de Walle, and J. S. Speck, *J. Vac. Sci. Technol. A* **35**, 041509 (2017). [doi: [10.1116/1.4986185](https://doi.org/10.1116/1.4986185)]
357. "First-principles characterization of native-defect-related optical transitions in ZnO", J. L. Lyons, J. B. Varley, D. Steiauf, A. Janotti and C. G. Van de Walle, *J. Appl. Phys.* **122**, 035704 (2017). [doi: [10.1063/1.4992128](https://doi.org/10.1063/1.4992128)]
358. "Deep donor state of the copper acceptor as a source of green luminescence in ZnO", J. L. Lyons, A. Alkauskas, A. Janotti and C. G. Van de Walle, *Appl. Phys. Lett.* **111**, 042101 (2017). [doi: [10.1063/1.4995404](https://doi.org/10.1063/1.4995404)]
359. "Lack of quantum confinement in Ga₂O₃ nanolayers", H. Peelaers and C.G. Van de Walle, *Phys. Rev. B* **96**, 081409(R) (2017). [doi: [10.1103/PhysRevB.96.081409](https://doi.org/10.1103/PhysRevB.96.081409)].
360. "Electronic and protonic conduction in LaFeO₃", Z. Zhu, H. Peelaers, and C. G. Van de Walle, *J. Mater. Chem. A* **5**, 15367 (2017). [doi: [10.1039/C7TA04330A](https://doi.org/10.1039/C7TA04330A)]
361. "Hole polarons and *p*-type doping in boron nitride polymorphs", L. Weston, D. Wickramaratne, and C. G. Van de Walle, *Phys. Rev. B* **96**, 100102(R) (2017). [doi: [10.1103/PhysRevB.96.100102](https://doi.org/10.1103/PhysRevB.96.100102)]
362. "Sub-band-gap absorption in Ga₂O₃", H. Peelaers and C. G. Van de Walle, *Appl. Phys. Lett.* **111**, 182104 (2017). [doi: [10.1063/1.5001323](https://doi.org/10.1063/1.5001323)]

363. “Band bowing and the direct-to-indirect crossover in random BAlN alloys”, J.-X. Shen, D. Wickramaratne, and C. G. Van de Walle, *Phys. Rev. Mater.* **1**, 065001 (2017) [doi: [10.1103/PhysRevMaterials.1.065001](https://doi.org/10.1103/PhysRevMaterials.1.065001)]
364. “Hybrid functional study of native point defects and impurities in ZnGeN₂”, N. L. Adamski, Z. Zhu, D. Wickramaratne, and C. G. Van de Walle, *J. Appl. Phys.* **122**, 195701 (2017). [doi: [10.1063/1.4999790](https://doi.org/10.1063/1.4999790)]
365. “Ultrawide-Bandgap Semiconductors: Research Opportunities and Challenges”, J. Y. Tsao, S. Chowdhury, M. A. Hollis, D. Jena, N. M. Johnson, K. A. Jones, R. J. Kaplar, S. Rajan, C. G. Van de Walle, E. Bellotti, C. L. Chua, R. Collazo, M. E. Coltrin, J. A. Cooper, K. R. Evans, S. Graham, T. A. Grotjohn, E. R. Heller, M. Higashiwaki, M. S. Islam, P. W. Juodawlkis, M. A. Khan, A. D. Koehler, J. H. Leach, U. K. Mishra, R. J. Nemanich, R. C. N. Pilawa-Podgurski, J. B. Shealy, Z. Sitar, M. J. Tadjer, A. F. Witulski, M. Wraback, J. A. Simmons, *Adv. Electron. Mater.* **4**, 1600501 (2018). [doi: [10.1002/aelm.201600501](https://doi.org/10.1002/aelm.201600501)]
366. “First-principles study of direct and indirect optical absorption in BaSnO₃”, Y. Kang, H. Peelaers, K. Krishnaswamy, and C. G. Van de Walle, *Appl. Phys. Lett.* **112**, 062106 (2018). [doi: [10.1063/1.5013641](https://doi.org/10.1063/1.5013641)]
367. “Comment on “Comparative study of *ab initio* nonradiative recombination rate calculations under different formalisms””, D. Wickramaratne, J.-X. Shen, A. Alkauskas, and C. G. Van de Walle, *Phys. Rev. B* **97**, 077301 (2018) [doi: [10.1103/PhysRevB.97.077301](https://doi.org/10.1103/PhysRevB.97.077301)]
368. “Interfacial cation-defect charge dipoles in stacked TiO₂-Al₂O₃ gate dielectrics”, L. Zhang, A. Janotti, A. C. Meng, K. Tang, C. G. Van de Walle, and P. C. McIntyre, *ACS Appl. Mater. Interfaces* **10**, 5140 (2018). [doi: [10.1021/acsami.7b19619](https://doi.org/10.1021/acsami.7b19619)]
369. “Origins of *n*-type doping difficulties in perovskite stannates”, L. Weston, L. Bjaalie, K. Krishnaswamy, and C. G. Van de Walle, *Phys. Rev. B* **97**, 054112 (2018). [doi: [10.1103/PhysRevB.97.054112](https://doi.org/10.1103/PhysRevB.97.054112)]
370. “Posner molecules: from atomic structure to nuclear spins”, M. W. Swift, C. G. Van de Walle, and M. P. A. Fisher, *Phys. Chem. Chem. Phys.* **20**, 12373 (2018). [doi: [10.1039/c7cp07720c](https://doi.org/10.1039/c7cp07720c)]
371. “Linear Hyperfine Tuning of Donor Spins in Silicon Using Hydrostatic Strain”, J. Mansir, P. Conti, Z. Zeng, J. J. Pla, P. Bertet, M. W. Swift, C. G. Van de Walle, M. L. W. Thewalt, B. Sklenard, Y. M. Niquet, and J. J. L. Morton, *Phys. Rev. Lett.* **120**, 167701 (2018). [doi: [10.1103/PhysRevLett.120.167701](https://doi.org/10.1103/PhysRevLett.120.167701)]
372. “Accurate and efficient band-offset calculations from density functional theory”, L. Weston, H. Taylor, K. Krishnaswamy, L. Bjaalie, and C. G. Van de Walle, *Comput. Mater. Sci.* **151**, 174 (2018). [doi: [10.1016/j.commatsci.2018.05.002](https://doi.org/10.1016/j.commatsci.2018.05.002)]

373. “Three-dimensional spin texture in hybrid perovskites and its impact on optical transitions”, X. Zhang, J.-X. Shen, and C. G. Van de Walle, *J. Phys. Chem. Lett.* **9**, 2903 (2018). [doi: [10.1021/acs.jpcllett.8b01004](https://doi.org/10.1021/acs.jpcllett.8b01004)]
374. “Structural and electronic properties of Ga₂O₃-Al₂O₃ alloys”, H. Peelaers, J. B. Varley, J. S. Speck, and C. G. Van de Walle, *Appl. Phys. Lett.* **112**, 242101 (2018) [doi: [10.1063/1.5036991](https://doi.org/10.1063/1.5036991)]; *ibid* **115**, 159901 (2019) (erratum). [doi: [10.1063/1.5127763](https://doi.org/10.1063/1.5127763)].
375. “Native point defects and impurities in hexagonal boron nitride”, L. Weston, D. Wickramaratne, M. Mackoite, A. Alkauskas, and C. G. Van de Walle, *Phys. Rev. B* **97**, 214104 (2018) [doi: [10.1103/PhysRevB.97.214104](https://doi.org/10.1103/PhysRevB.97.214104)]; **102**, 099903 (2020) (erratum) [doi: [10.1103/PhysRevB.102.099903](https://doi.org/10.1103/PhysRevB.102.099903)].
376. “Electron doping in Sr₃Ir₂O₇: Collapse of band gap and magnetic order”, M. W. Swift, Z. Porter, S. D. Wilson, and C. G. Van de Walle, *Phys. Rev. B* **98**, 081106(R) (2018). [doi: [10.1103/PhysRevB.98.081106](https://doi.org/10.1103/PhysRevB.98.081106)]
377. “First-principles analysis of radiative recombination in lead-halide perovskites”, X. Zhang, J.-X. Shen, W. Wang, and C. G. Van de Walle, *ACS Energy Lett.* **3**, 2329 (2018). [doi: [10.1021/acscenergylett.8b01297](https://doi.org/10.1021/acscenergylett.8b01297)]
378. “Ion-Transport Engineering of Alkaline-Earth Hydrides for Hydride Electrolyte Applications”, A. J. E. Rowberg, L. Weston, and C. G. Van de Walle, *Chem. Mater.* **30**, 5878 (2018). [doi: [10.1021/acs.chemmater.8b01593](https://doi.org/10.1021/acs.chemmater.8b01593)]
379. “Unexpectedly strong Auger recombination in halide perovskites”, J.-X. Shen, X. Zhang, S. Das, E. Kioupakis, and C. G. Van de Walle, *Adv. Energy Mater.* **8**, 1801027 (2018). [doi: [10.1002/aenm.201801027](https://doi.org/10.1002/aenm.201801027)]
380. “Carrier-induced absorption as a mechanism for electrochromism in WO₃”, W. Wang, H. Peelaers, J. X. Shen, and C. G. Van de Walle, *MRS Commun.* **8**, 926 (2018). [doi: [10.1557/mrc.2018.115](https://doi.org/10.1557/mrc.2018.115)]
381. “Sr₃Ir₂O₇F₂: Topochemical conversion of a relativistic Mott state into a spin-orbit driven band insulator”, C. Peterson, M. W. Swift, Z. Porter, R. J. Clément, G. Wu, G. H. Ahn, S. J. Moon, B. C. Chakoumakos, J. P. C. Ruff, H. Cao, C. Van de Walle and S. D. Wilson, *Phys. Rev. B* **98**, 155128 (2018). [doi: [10.1103/PhysRevB.98.155128](https://doi.org/10.1103/PhysRevB.98.155128)]
382. “Defect identification based on first-principles calculations for deep level transient spectroscopy”, D. Wickramaratne, C. E. Dreyer, B. Monserrat, J.-X. Shen, J. L. Lyons, A. Alkauskas, and C. G. Van de Walle, *Appl. Phys. Lett.* **113**, 192106 (2018). [doi: [10.1063/1.5047808](https://doi.org/10.1063/1.5047808)]
383. “Monolayer to bulk properties of hexagonal boron nitride”, D. Wickramaratne, L. Weston, and C. G. Van de Walle, *J. Phys. Chem. C* **122**, 25524 (2018). [doi: [10.1021/acs.jpcc.8b09087](https://doi.org/10.1021/acs.jpcc.8b09087)]

384. “Deep acceptors and their diffusion in Ga₂O₃”, H. Peelaers, J. L. Lyons, J. B. Varley, and C. G. Van de Walle, *APL Materials* **7**, 022519 (2019). [doi: [10.1063/1.5063807](https://doi.org/10.1063/1.5063807)]
385. “Strategies for *p*-type doping of ZnGeN₂”, N. L. Adamski, Z. Zhu, D. Wickramaratne, and C. G. Van de Walle, *Appl. Phys. Lett.* **114**, 032101 (2019). [doi: [10.1063/1.5063581](https://doi.org/10.1063/1.5063581)]
386. “Optimizing proton conductivity in zirconates through defect engineering”, A. J. E. Rowberg, L. Weston, and C. G. Van de Walle, *ACS Appl. Ener. Mater.* **2**, 2611 (2019). [doi: [10.1021/acsaem.8b02222](https://doi.org/10.1021/acsaem.8b02222)]
387. “Electrical and optical properties of iron in GaN, AlN, and InN”, D. Wickramaratne, J.-X. Shen, C.E. Dreyer, A. Alkauskas, and C. G. Van de Walle, *Phys. Rev. B* **99**, 205202 (2019). [doi: [10.1103/PhysRevB.99.205202](https://doi.org/10.1103/PhysRevB.99.205202)]
388. “Hydrogen-induced degradation of NaMnO₂”, Z. Zhu, H. Peelaers, and C. G. Van de Walle, *Chem. Mater.* **31**, 5224 (2019). [doi: [10.1021/acs.chemmater.9b01458](https://doi.org/10.1021/acs.chemmater.9b01458)]
389. “Phonon- and charged-impurity-assisted indirect free-carrier absorption in Ga₂O₃”, H. Peelaers and C. G. Van de Walle, *Phys. Rev. B* **100**, 081202(R) (2019). [doi: [10.1103/PhysRevB.100.081202](https://doi.org/10.1103/PhysRevB.100.081202)]
390. “Role of point defects in the electrical and optical properties of In₂O₃”, I. Chatratin, F. P. Sabino, P. Reunchan, S. Limpijumnong, J. B. Varley, C. G. Van de Walle, and A. Janotti, *Phys. Rev. Mater.* **3**, 074604 (2019). [doi: [10.1103/PhysRevMaterials.3.074604](https://doi.org/10.1103/PhysRevMaterials.3.074604)]
391. “Limitations of In₂O₃ as a transparent conducting oxide”, H. Peelaers, E. Kioupakis, and C. G. Van de Walle, *Appl. Phys. Lett.* **115**, 082105 (2019) [doi: [10.1063/1.5109569](https://doi.org/10.1063/1.5109569)]
392. “Dangling bonds in hexagonal boron nitride as single-photon emitters”, M. E. Turiansky, A. Alkauskas, L. C. Bassett, and C. G. Van de Walle, *Phys. Rev. Lett.* **123**, 127401 (2019). [doi: [10.1103/PhysRevLett.123.127401](https://doi.org/10.1103/PhysRevLett.123.127401)]
393. “First-principles study of bandgap bowing in B GaN alloys”, M. E. Turiansky, J.-X. Shen, D. Wickramaratne, and C. G. Van de Walle, *J. Appl. Phys* **126**, 095706 (2019). [doi: [10.1063/1.5111414](https://doi.org/10.1063/1.5111414)]
394. “First-principles study of electron-phonon interactions and transport in anatase TiO₂”, Y. Kang, H. Peelaers, and C. G. Van de Walle, *Phys. Rev. B* **100**, 121113(R) (2019). [doi: [10.1103/PhysRevB.100.121113](https://doi.org/10.1103/PhysRevB.100.121113)]
395. “Optimizing *n*-type doping of ZnGeN₂ and ZnSiN₂”, N. L. Adamski, Z. Zhu, D. Wickramaratne, and C. G. Van de Walle, *Phys. Rev. B* **100**, 155206 (2019). [doi: [10.1103/PhysRevB.100.155206](https://doi.org/10.1103/PhysRevB.100.155206)]
396. “Unusual formation of point defect complexes in the ultra-wide band gap semiconductor β-Ga₂O₃”, J. M. Johnson, Z. Chen, J. B. Varley, C. M. Jackson, E. Farzana, Z. Zhang, A. R. Arehart, H.-L. Huang, A. Genc, S. A. Ringel, C. G. Van de Walle, D. A. Muller, and J. Hwang, *Phys. Rev. X* **9**, 041027 (2019). [doi: [10.1103/PhysRevX.9.041027](https://doi.org/10.1103/PhysRevX.9.041027)]

397. “First-principles study of antisite defects in perovskite stannates”, S. KC, A. J. E. Rowberg, L. Weston, and C. G. Van de Walle, *J. Appl. Phys.* **126**, 195701 (2019). [doi: [10.1063/1.5126206](https://doi.org/10.1063/1.5126206)]
398. “Impact of phonons and spin-orbit coupling on Auger recombination in InAs”, J.-X. Shen, D. Steiauf, A. McAllister, G. Shi, E. Kioupakis, A. Janotti, and C. G. Van de Walle, *Phys. Rev. B* **100**, 155202 (2019). [doi: [10.1103/PhysRevB.100.155202](https://doi.org/10.1103/PhysRevB.100.155202)]
399. “Carbon dimer defect as a source of the 4.1 eV luminescence in hexagonal boron nitride”, M. Mackoite-Sinkevičienė, M. Maciaszek, C. G. Van de Walle, and A. Alkauskas, *Appl. Phys. Lett.* **115**, 212101 (2019). [doi: [10.1063/1.5124153](https://doi.org/10.1063/1.5124153)]
400. “Deep-Level Defects and Impurities in InGaN Alloys”, D. Wickramaratne, C. E. Dreyer, J.-X. Shen, J. L. Lyons, A. Alkauskas, and C. G. Van de Walle, *Phys. Stat. Solidi B* **257**, 1900534 (2019). [doi: [10.1002/pssb.201900534](https://doi.org/10.1002/pssb.201900534)]
401. “Giant polarization charge density at lattice-matched GaN/ScN interfaces”, N. L. Adamski, C. E. Dreyer, and C. G. Van de Walle, *Appl. Phys. Lett.* **115**, 232103 (2019). [doi: [10.1063/1.5126717](https://doi.org/10.1063/1.5126717)]
402. “*Ab initio* study of enhanced thermal conductivity in ordered AlGaO₃ alloys”, S. Mu, H. Peelaers, and C. G. Van de Walle, *Appl. Phys. Lett.* **115**, 242103 (2019). [doi: [10.1063/1.5131755](https://doi.org/10.1063/1.5131755)]
403. “First-principles simulation of carrier recombination mechanisms in halide perovskites”, X. Zhang, J.-X. Shen, and C. G. Van de Walle, *Adv. Energy Mater.* **10**, 1902830 (2020). [doi: [10.1002/aenm.201902830](https://doi.org/10.1002/aenm.201902830)]
404. “First-principles study of transport in WO₃”, W. Wang, Y. Kang, H. Peelaers, K. Krishnaswamy, and C. G. Van de Walle, *Phys. Rev. B* **101**, 045116 (2020). [doi: [10.1103/PhysRevB.101.045116](https://doi.org/10.1103/PhysRevB.101.045116)]
405. “Effect of Titanium Induced Chemical Inhomogeneity on Crystal Structure, Electronic Structure and Optical Properties of Wide Band Gap Ga₂O₃”, M. Bandi, V. Zade, S. Roy, A. N. Nair, S. Seacat, S. Sreenivasan, V. Shutthanandan, C. G. Van de Walle, H. Peelaers, and C. V. Ramana, *Cryst. Growth Des.* **20**, 1422 (2020) [doi: [10.1021/acs.cgd.9b00747](https://doi.org/10.1021/acs.cgd.9b00747)]
406. “Correctly assessing defect tolerance in halide perovskites”, X. Zhang, M. E. Turiansky, and C. G. Van de Walle, *J. Phys. Chem. C* **124**, 6022 (2020). [doi: [10.1021/acs.jpcc.0c01324](https://doi.org/10.1021/acs.jpcc.0c01324)]
407. “Iodine interstitials as a cause of nonradiative recombination in hybrid perovskites”, X. Zhang, M. E. Turiansky, J.-X. Shen, and C. G. Van de Walle, *Phys. Rev. B* **101**, 140101(R) (2020). [doi: [10.1103/PhysRevB.101.140101](https://doi.org/10.1103/PhysRevB.101.140101)]
408. “Spinning up quantum defects in 2D materials”, M. E. Turiansky, A. Alkauskas, and C. G. Van de Walle, *Nat. Mater.* **19**, 487 (2020). [doi: [10.1038/s41563-020-0668-x](https://doi.org/10.1038/s41563-020-0668-x)]

409. “Band alignments and polarization properties of the Zn-IV-nitrides”, N. L. Adamski, D. Wickramaratne, and C. G. Van de Walle, *J. Mater. Chem. C*, **8**, 7890 (2020). [doi: [10.1039/d0tc01578d](https://doi.org/10.1039/d0tc01578d)]
410. “Anomalous Auger recombination in PbSe”, X. Zhang, J.-X. Shen, and C. G. Van de Walle, *Phys. Rev. Lett.* **125**, 037401 (2020). [doi: [10.1103/PhysRevLett.125.037401](https://doi.org/10.1103/PhysRevLett.125.037401)]
411. “Hidden role of Bi incorporation in nonradiative recombination in methylammonium lead iodide”, X. Zhang, J.-X. Shen, M. E. Turiansky, and C. G. Van de Walle, *J. Mater. Chem. A*, **8**, 12964 (2020). [doi: [10.1039/d0ta04968a](https://doi.org/10.1039/d0ta04968a)]
412. “Prospects for high carrier mobility in the cubic germanates”, A. J. E. Rowberg, K. Krishnaswamy, and C. G. Van de Walle, *Semicond. Sci. Technol.* **35**, 085030 (2020). [doi: [10.1088/1361-6641/ab97f6](https://doi.org/10.1088/1361-6641/ab97f6)]
413. “Role of Ga and In adatoms in the epitaxial growth of β -Ga₂O₃”, M. Wang, S. Mu, and C. G. Van de Walle, *Phys. Rev. B* **102**, 035303 (2020). [doi: [10.1103/PhysRevB.102.035303](https://doi.org/10.1103/PhysRevB.102.035303)]
414. “Radiative capture rates at deep defects from electronic structure calculations”, C. E. Dreyer, A. Alkauskas, J. L. Lyons, and C. G. Van de Walle, *Phys. Rev. B* **102**, 085305 (2020). [doi: [10.1103/PhysRevB.102.085305](https://doi.org/10.1103/PhysRevB.102.085305)]
415. “First-principles surface energies for monoclinic Ga₂O₃ and Al₂O₃ and consequences for cracking of (Al_xGa_{1-x})₂O₃”, S. Mu, M. Wang, H. Peelaers, and C. G. Van de Walle, *APL Mater.* **8**, 091105 (2020). [doi: [10.1063/5.0019915](https://doi.org/10.1063/5.0019915)]
416. “Electronic structure and magneto-optical properties of silicon-nitrogen-vacancy complexes in diamond”, M. R. Zemła, K. Czelej, P. Kamińska, C. G. Van de Walle, and J. A. Majewski, *Phys. Rev. B* **102**, 115102 (2020). [doi: [10.1103/PhysRevB.102.115102](https://doi.org/10.1103/PhysRevB.102.115102)]
417. “Inflection points in the conduction-band structure of BaSnO₃”, A. J. E. Rowberg, K. Krishnaswamy, and C. G. Van de Walle, *Phys. Rev. B* **102**, 115201 (2020). [doi: [10.1103/PhysRevB.102.115201](https://doi.org/10.1103/PhysRevB.102.115201)]
418. “First-principles calculations of hyperfine interaction, binding energy, and quadrupole coupling for shallow donors in silicon”, M. W. Swift, H. Peelaers, S. Mu, J. J. L. Morton, and C. G. Van de Walle, *NPJ Comput. Mater.* **6**, 181 (2020). [doi: [10.1038/s41524-020-00448-7](https://doi.org/10.1038/s41524-020-00448-7)]
419. “Polarization properties at rocksalt/wurtzite oxide interfaces”, N. L. Adamski, C. E. Dreyer, and C. G. Van de Walle, *Phys. Rev. B* **102**, 201301 (2020) (R). [doi: [10.1103/PhysRevB.102.201301](https://doi.org/10.1103/PhysRevB.102.201301)]
420. “Orientation-dependent band offsets between (Al_xGa_{1-x})₂O₃ and Ga₂O₃”, S. Mu, H. Peelaers, Y. Zhang, M. Wang, and C. G. Van de Walle, *Appl. Phys. Lett.* **117**, 252104 (2020). [doi: [10.1063/5.0036072](https://doi.org/10.1063/5.0036072)]

421. "Defect chemistry and hydrogen transport in La/Sr-based oxyhydrides", A. J. E. Rowberg, L. Weston, and C. G. Van de Walle, *J. Phys. Chem. C* **125**, 2250 (2021). [doi: <https://doi.org/10.1021/acs.jpcc.0c09222>]
422. "Boron dangling bonds in a monolayer of hexagonal boron nitride", M. E. Turiansky and C. G. Van de Walle, *J. Appl. Phys.* **129**, 064301 (2021). [doi: [10.1063/5.0040780](https://doi.org/10.1063/5.0040780)]
423. "Impact of dangling bonds on properties of h-BN", M. E. Turiansky and C. G. Van de Walle, *2D Mater.* **8**, 024002 (2021). [doi: [10.1088/2053-1583/abe4bb](https://doi.org/10.1088/2053-1583/abe4bb)]
424. "Adsorption and diffusion of aluminum on β -Ga₂O₃ (010) surfaces", M. Wang, S. Mu, and C. G. Van de Walle, *ACS Appl. Mater. Interfaces* **13**, 10650 (2021). [doi: [10.1021/acsami.0c22737](https://doi.org/10.1021/acsami.0c22737)]
425. "Thermodynamics of boron incorporation in B GaN", J.-X. Shen, M. E. Turiansky, D. Wickramaratne, and C. G. Van de Walle, *Phys. Rev. Mater.* **5**, L030401 (2021). [doi: [10.1103/PhysRevMaterials.5.L030401](https://doi.org/10.1103/PhysRevMaterials.5.L030401)]
426. "A first-principles understanding of point defects and impurities in GaN", J. L. Lyons, D. Wickramaratne, and C. G. Van de Walle, *J. Appl. Phys.* **129**, 111101 (2021). [doi: [10.1063/5.0041506](https://doi.org/10.1063/5.0041506)]
427. "Atomic scale investigation of aluminum incorporation, defects, and phase stability in β -(Al_xGa_{1-x})₂O₃", J. M. Johnson, H.-L. Huang, M. Wang, S. Mu, J. B. Varley, A. F. M. A. U. Bhuiyan, Z. Feng, N. K. Kalarickal, S. Rajan, H. Zhao, C. G. Van de Walle, and J. Hwang, *APL Mater.* **9**, 051103 (2021). [doi: [10.1063/5.0039769](https://doi.org/10.1063/5.0039769)]
428. "Finite-size correction for slab supercell calculations of materials with spontaneous polarization", S. H. Yoo, M. Todorova, D. Wickramaratne, L. Weston, C. G. Van de Walle, and J. Neugebauer, *npj Comput. Mater.* **7**, 58 (2021). [doi: [10.1038/s41524-021-00529-1](https://doi.org/10.1038/s41524-021-00529-1)]
429. "Nonrad: Computing nonradiative capture coefficients from first principles", M. E. Turiansky, A. Alkauskas, M. Engel, G. Kresse, D. Wickramaratne, J.-X. Shen, C. E. Dreyer, and C. G. Van de Walle, *Comput. Phys. Commun.* **267**, 108056 (2021). [doi: [10.1016/j.cpc.2021.108056](https://doi.org/10.1016/j.cpc.2021.108056)]
430. "Minimizing hydrogen vacancies to enable highly efficient hybrid perovskites", X. Zhang, J.-X. Shen, M. E. Turiansky, and C. G. Van de Walle, *Nat. Mater.* **20**, 971 (2021). [doi: [10.1038/s41563-021-00986-5](https://doi.org/10.1038/s41563-021-00986-5)]
431. "Hole trapping at acceptor impurities and alloying elements in AlN", J. L. Lyons and C. G. Van de Walle, *Phys. Status Solidi RRL* **15**, 2100218 (2021). [doi: [10.1002/pssr.202100218](https://doi.org/10.1002/pssr.202100218)]
432. "Vibrational and vibronic structure of isolated point defects: the nitrogen-vacancy center in diamond", L. Razinkovas, M. W. Doherty, N. B. Manson, C. G. Van de Walle, and A. Alkauskas, *Phys. Rev. B* **104**, 045303 (2021). [doi: [10.1103/PhysRevB.104.045303](https://doi.org/10.1103/PhysRevB.104.045303)]

433. “Understanding carbon contamination in the proton-conducting zirconates and cerates”, A. J. E. Rowberg, M. W. Swift, and C. G. Van de Walle, *Phys. Chem. Chem. Phys.* **23**, 14205 (2021). [doi: [10.1039/D1CP01902C](https://doi.org/10.1039/D1CP01902C)]
434. “Hydride conductivity in nitride hydrides”, A. J. E. Rowberg and C. G. Van de Walle, *ACS Appl. Energy Mater.* **4**, 6348 (2021). [doi: [10.1021/acsaem.1c01208](https://doi.org/10.1021/acsaem.1c01208)]
435. “Materials and device simulations for silicon qubit design and optimization”, M. F. Gyure, A. A. Kiselev, R. S. Ross, R. Rahman, and C. G. Van de Walle, *MRS Bull.* **46**, 634 (2021). [doi: [10.1557/s43577-021-00140-1](https://doi.org/10.1557/s43577-021-00140-1)]
436. “First-principles study of electron transport in ScN”, S. Mu, A. J. E. Rowberg, J. Leveillee, F. Giustino, and C. G. Van de Walle, *Phys. Rev. B* **104**, 075118 (2021). [doi: [10.1103/PhysRevB.104.075118](https://doi.org/10.1103/PhysRevB.104.075118)]
437. “Structural, electronic, and polarization properties of YN and LaN”, A. J. E. Rowberg, S. Mu, M. W. Swift, and C. G. Van de Walle, *Phys. Rev. Mater.* **5**, 094602 (2021). [doi: [10.1103/PhysRevMaterials.5.094602](https://doi.org/10.1103/PhysRevMaterials.5.094602)]
438. “Piezoelectric effect and polarization switching in $\text{Al}_{1-x}\text{Sc}_x\text{N}$ ”, H. Wang, N. Adamski, S. Mu, and C. G. Van de Walle, *J. Appl. Phys.* **130**, 104101 (2021). [doi: [10.1063/5.0056485](https://doi.org/10.1063/5.0056485)]
439. “All-inorganic halide perovskites as candidates for efficient solar cells”, X. Zhang, M. E. Turiansky, and C. G. Van de Walle, *Cell Rep. Phys. Sci.* **2**, 100604 (2021). [doi: [10.1016/j.xcrp.2021.100604](https://doi.org/10.1016/j.xcrp.2021.100604)]
440. “Prospects for *n*-type conductivity in cubic boron nitride”, M. E. Turiansky, D. Wickramaratne, J. L. Lyons, and C. G. Van de Walle, *Appl. Phys. Lett.* **119**, 162105 (2021). [doi: [10.1063/5.0069970](https://doi.org/10.1063/5.0069970)]
441. “Surprising stability of the polar (001) surface of the Mott insulator GdTiO_3 ”, K. Krishnaswamy, A. Janotti, L. Bjaalie, and C. G. Van de Walle, *J. Vac. Sci. Technol. A* **39**, 063220 (2021). [doi: [10.1116/6.0001313](https://doi.org/10.1116/6.0001313)]
442. “Incorporation of Si and Sn donors in $\beta\text{-Ga}_2\text{O}_3$ through surface reconstructions”, M. Wang, S. Mu, and C. G. Van de Walle, *J. Appl. Phys.* **130**, 185703 (2021). [doi: [10.1063/5.0068875](https://doi.org/10.1063/5.0068875)]
443. “Mg doping and diffusion in (010) $\beta\text{-Ga}_2\text{O}_3$ films grown by plasma-assisted molecular beam epitaxy”, A. Mauze, Y. Zhang, T. Itoh, T. Mates, H. Peelaers, C. G. Van de Walle, and J. S. Speck, *J. Appl. Phys.* **130**, 235301 (2021). [doi: [10.1063/5.0072611](https://doi.org/10.1063/5.0072611)]

BOOK CHAPTERS

1. “Theory of isolated interstitial hydrogen and muonium in crystalline semiconductors”, C.

- G. Van de Walle, in *Hydrogen in Semiconductors*, edited by J. I. Pankove and N. M. Johnson, *Semiconductors and Semimetals*, Vol. 34, Treatise Editors R. K. Willardson and A. C. Beer (Academic Press, Boston, 1991), p. 585.
2. “Hydrogen in crystalline semiconductors”, C. G. Van de Walle, in *Deep Centers in Semiconductors*, 2nd edition, edited by S. T. Pantelides (Gordon and Breach Science Publishers, Philadelphia, 1992), p. 899.
 3. “First-principles calculations of light emission from silicon-based materials”, C. G. Van de Walle and J. E. Northrup, in *Porous Silicon*, edited by Z. C. Feng and R. Tsu (World Scientific Publishing Co. Inc, Singapore, 1994), p. 329.
 4. “Doping of wide-band-gap II-VI semiconductors - Theory”, C. G. Van de Walle, in *II-VI pn junction blue/green light emitters*, edited by R. L. Gunshor and A. Nurmikko, *Semiconductors and Semimetals*, Vol. 44, Treatise Editors R. K. Willardson and A. C. Beer (Academic Press, Boston, 1997), p. 121.
 5. “Hydrogen in III-V nitrides”, C. G. Van de Walle and N. M. Johnson, in *Gallium Nitride (GaN) II*, edited by J. I. Pankove and T. D. Moustakas, *Semiconductors and Semimetals*, Vol. 57, Treatise Editors R. K. Willardson and E. R. Weber (Academic Press, Boston, 1998), p. 157.
 6. “Hydrogen interaction with polycrystalline and amorphous silicon – theory”, C. G. Van de Walle, in *Hydrogen in Semiconductors II*, edited by N. H. Nickel, *Semiconductors and Semimetals*, Vol. 61, Treatise Editors R. K. Willardson and E. R. Weber (Academic Press, Boston, 1999), p. 241.
 7. “Theory of hydrogen in GaN”, J. Neugebauer and C. G. Van de Walle, in *Hydrogen in Semiconductors II*, edited by N. H. Nickel, *Semiconductors and Semimetals*, Vol. 61, Treatise Eds. R. K. Willardson and E. R. Weber (Academic Press, Boston, 1999), p. 479.
 8. “Isolated monatomic hydrogen in silicon”, N. M. Johnson and C. G. Van de Walle, in *Hydrogen in Semiconductors II*, edited by N. H. Nickel, *Semiconductors and Semimetals*, Vol. 61, Treatise Editors R. K. Willardson and E. R. Weber (Academic Press, Boston, 1999), p. 13.
 9. “Electrical Conductivity Control”, C. G. Van de Walle, Chapter 3 in *Introduction to Nitride Semiconductor Blue Lasers and Light Emitting Diodes*, edited by S. Nakamura and S. F. Chichibu (Taylor and Francis, London, 2000), pp. 67-103.
 10. “Theory of native point defects and impurities in InN”, A. Janotti and C. G. Van de Walle, Chapter 11 in *Indium Nitride and Related Alloys*, edited by T. D. Veal, C. F. McConville, and W. J. Schaff (CRC Press, Boca Raton, 2010), pp. 419-444.
 11. “Theory of InN surfaces”, C. G. Van de Walle, Chapter 13 in *Indium Nitride and Related Alloys*, edited by T. D. Veal, C. F. McConville, and W. J. Schaff (CRC Press, Boca Raton, 2010), pp. 497-513.

12. “Native Point Defects and Doping in ZnO”, A. Janotti and C. G. Van de Walle, Chapter 5 in *Zinc Oxide Materials for Electronic and Optoelectronic Device Applications*, edited by C. W. Litton, T. C. Collins, and D. C. Reynolds, Wiley Series in Materials for Electronic & Optoelectronic Applications, Series Eds. P. Capper, S. Kasap, and A. Willoughby (John Wiley & Sons, Chichester, 2011), pp. 113-134.
13. “Advances in Electronic Structure Methods for Defects and Impurities in Solids”, C. G. Van de Walle and A. Janotti, Chapter 1 in *Advanced Calculations for Defects in Materials: Electronic Structure Methods*, edited by A. Alkauskas, P. Deák, J. Neugebauer, A. Pasquarello, and C. G. Van de Walle (Wiley-VCH, Weinheim, 2011), pp. 1-16.
14. “LDA+*U* and Hybrid Functional Calculations for Defects in ZnO, SnO₂, and TiO₂”, A. Janotti and C. G. Van de Walle, Chapter 9 in *Advanced Calculations for Defects in Materials: Electronic Structure Methods*, edited by A. Alkauskas, P. Deák, J. Neugebauer, A. Pasquarello, and C. G. Van de Walle (Wiley-VCH, Weinheim, 2011), pp. 155-164.
15. “Electrostatic Interactions between Charged Defects in Supercells”, C. Freysoldt, J. Neugebauer, and C. G. Van de Walle, Chapter 14 in *Advanced Calculations for Defects in Materials: Electronic Structure Methods*, edited by A. Alkauskas, P. Deák, J. Neugebauer, A. Pasquarello, and C. G. Van de Walle (Wiley-VCH, Weinheim, 2011), pp. 241-258.
16. “Controlling the Conductivity in Oxide Semiconductors”, A. Janotti, J. B. Varley, J. L. Lyons, and C. G. Van de Walle, in *Functional Metal Oxide Semiconductors*, edited by J. Wu, J. Cao, W.-Q. Han, A. Janotti, and H.-C. Kim, Springer Series in Materials Science, Vol. 149 (Springer, New York, 2011), pp. 23-36.
17. “Energy Conversion: Solid-State Lighting”, E. Kioupakis, P. Rinke, A. Janotti, Q. Yan, and C. G. Van de Walle, Chapter 8 in *Computational Approaches to Energy Materials*, edited by A. Walsh, A. A. Sokol and C. R. A. Catlow (John Wiley & Sons Ltd, Oxford, UK, 2013). [doi: 10.1002/9781118551462.ch8]
18. “Theory and modeling of oxide semiconductors,” J. L. Lyons, A. Janotti, and C. G. Van de Walle, in *Oxide Semiconductors*, edited by B. G. Svensson, S. J. Pearton, and C. Jagadish, *Semiconductors and Semimetals* vol. 88 (Academic Press, Burlington, 2013). [doi:10.1016/B978-0-12-396489-2.00001-1]
19. “Defects in germanium”, J. Weber, A. Janotti, and C. G. Van de Walle, Chapter 1 in *Photonics and Electronics with Germanium*, edited by K. Wada and L. C. Kimerling (Wiley-VCH, Weinheim, 2015), pp. 1-23.
20. “Point Defects and Impurities in III-Nitride Bulk and Thin Film Heterostructures”, C. E. Dreyer and C. G. Van de Walle, in *Reference Module in Materials Science and Materials Engineering*, edited by S. Hashmi (Elsevier, Oxford, 2016), pp. 1-8.

21. “First-Principles Calculations 1—Electronic and structural properties of Ga₂O₃ and alloys with In₂O₃ and Al₂O₃”, H. Peelaers and C. G. Van de Walle, in *Gallium Oxide—Materials Properties, Crystal Growth, and Devices*, eds. M. Higashiwaki and S. Fujita (Springer Nature Switzerland AG, 2020), p. 309. [doi: [10.1007/978-3-030-37153-1](https://doi.org/10.1007/978-3-030-37153-1)]

REVIEW ARTICLES

1. “Strain effects on the valence-band structure of SiGe”; “Strain effects on the conduction-band structure of SiGe”; “SiGe heterojunctions and band offsets”; C. G. Van de Walle, in *Properties of Strained and Relaxed SiGe*, edited by E. Kasper, EMIS Datareview Series No. 12 (INSPEC, IEE, 1995), pp. 94-98, 99-102, 110-115.
2. “Condensed-Matter Physics”, C. G. Van de Walle, in *1995 Yearbook of Science and the Future*, edited by David Calhoun (Encyclopaedia Britannica, Chicago, 1994), p.405.
3. “Heterojunction band offset engineering”, A. Franciosi and C. G. Van de Walle, Surf. Sci. Rep. **25**, 1 (1996). [doi: [10.1016/0167-5729\(95\)00008-9](https://doi.org/10.1016/0167-5729(95)00008-9)]
4. “Native defects, impurities, and doping in GaN and related compounds: general remarks”; “Native point defects in GaN and related compounds”; “Yellow luminescence in GaN”; “Hydrogen and acceptor compensation in GaN”; C. G. Van de Walle *et al.*, in *Properties, Processing and Applications of Gallium Nitride and Related Semiconductors*, edited by J. Edgar, S. Strite, I. Akasaki, H. Amano, and C. Wetzel, EMIS Datareview Series No. 23 (INSPEC, IEE, 1999), pp. 275-280; 281-283; 313-316; 317-321.
5. “Strain effects on the valence-band structure of SiGe”; “Strain effects on the conduction-band structure of SiGe”; “SiGe heterojunctions and band offsets”; C. G. Van de Walle, in *Properties of Silicon Germanium and SiGe: Carbon*, edited by E. Kasper and K. Lyutovich, EMIS Datareview Series No. 24 (INSPEC, IEE, 2000), pp. 135-139, 140-143, 149-157.
6. “Point Defects and Impurities in III-Nitride Bulk and Thin Film Heterostructures”, C. G. Van de Walle, in *Encyclopedia of Materials: Science and Technology* Vol. 7, 7124 (Pergamon, Amsterdam, 2001).
7. “First-principles calculations for defects and impurities: Applications to III-nitrides” (Applied Physics Review), C. G. Van de Walle and J. Neugebauer, J. Appl. Phys. **95**, 3851 (2004). [doi: [10.1063/1.1682673](https://doi.org/10.1063/1.1682673)]
8. “Defects and Impurities in Semiconductors”, C. G. Van de Walle, in *Handbook of Materials Modeling*, edited by S. Yip (Springer, 2005), pp. 1877-1888.
9. “Hydrogen in semiconductors”, C. G. Van de Walle and J. Neugebauer, Annu. Rev. Mater. Res. **36**, 179 (2006). [doi: [10.1146/annurev.matsci.36.010705.155428](https://doi.org/10.1146/annurev.matsci.36.010705.155428)]
10. “Fundamentals of zinc oxide as a semiconductor”, A. Janotti and C. G. Van de Walle, Rep. Prog. Phys. **72**, 126501 (2009). [doi: [10.1088/0034-4885/72/12/126501](https://doi.org/10.1088/0034-4885/72/12/126501)]

11. “First-principles calculations for point defects in solids”, C. Freysoldt, B. Grabowski, T. Hickel, J. Neugebauer, G. Kresse, A. Janotti, and C. G. Van de Walle, *Rev. Mod. Phys.* **86**, 253 (2014). [doi: [10.1103/RevModPhys.86.253](https://doi.org/10.1103/RevModPhys.86.253)]
12. “First-Principles Calculations of Point Defects for Quantum Technologies”, C. E. Dreyer, A. Alkauskas, J. L. Lyons, A. Janotti, and C. G. Van de Walle, *Annu. Rev. Mater. Res.* **48**, 1 (2018). [doi: [10.1146/annurev-matsci-070317-124453](https://doi.org/10.1146/annurev-matsci-070317-124453)]

DISSERTATION

“Theoretical studies of structure and band alignment at semiconductor interfaces”, C. G. Van de Walle, Ph. D. Dissertation, Stanford University (1986).

BOOKS EDITED

1. *Advanced Calculations for Defects in Materials: Electronic Structure Methods*, edited by A. Alkauskas, P. Deák, J. Neugebauer, A. Pasquarello, and C. G. Van de Walle (Wiley-VCH, Weinheim, 2011).

CONFERENCE PROCEEDINGS EDITED

1. *Wide-Band-Gap Semiconductors: Proceedings of the Seventh Trieste Semiconductor Symposium*, Trieste, Italy, June 8-12, 1992, edited by C. G. Van de Walle (*Physica B*, volume 185) (North-Holland, Elsevier Science Publishers, Amsterdam, 1993).
2. *Proceedings of the 20th International Conference on Defects in Semiconductors*, Berkeley, California, July 26-30, 1999, edited by C. G. Van de Walle and W. Walukiewicz (*Physica B*, volume 273-274) (North-Holland, Elsevier Science, Amsterdam, 1999).
3. *Proceedings of the 27th International Conference on the Physics of Semiconductors*, Flagstaff, Arizona, July 26-30, 2004, edited by J. Menéndez and C. G. Van de Walle (*AIP Conference Proceedings Vol. 772*) (American Institute of Physics, Melville, NY, 2005).

CONFERENCE PROCEEDINGS PAPERS

1. “Theoretical study of semiconductor interfaces”, C. G. Van de Walle and R. M. Martin, in *Computer-Based Microscopic Description of the Structure and Properties of Materials*, edited by J. Broughton, W. Krakow and S. T. Pantelides, *Materials Research Society Symposia Proceedings*, Vol. 63 (Materials Research Society, Pittsburgh, Pennsylvania, 1986), p. 21.
2. “A simple model for intrinsic band offsets at semiconductor heterojunctions”, C. G. Van de Walle and R. M. Martin, in *Proceedings of the 18th International Conference on the Physics of Semiconductors*, edited by O. Engström (World Scientific Publishing Co Pte Ltd., Singapore 1987), p. 159.

3. "Energy-dependence of the single-particle self-energy correction for various semiconductors", W. B. Jackson, C. G. Van de Walle, J. W. Allen, and J. E. Northrup, in *Proceedings of the 18th International Conference on the Physics of Semiconductors*, edited by O. Engström (World Scientific Publishing Co Pte Ltd., Singapore 1987), p. 1111.
4. "Band offsets at strained-layer interfaces", C. G. Van de Walle, in *Epitaxy of Semiconductor Layered Structures*, edited by R. T. Tung, L. R. Dawson, and R. L. Gunshor, Materials Research Society Symposia Proceedings, Vol. 102 (Materials Research Society, Pittsburgh, Pennsylvania, 1988), p. 565.
5. "Theory of hydrogen reactions in silicon", C. G. Van de Walle, Y. Bar-Yam, and S. T. Pantelides, in *Defects in Electronic Materials*, edited by M. Stavola, S. J. Pearton, and G. Davies, Materials Research Society Symposia Proceedings, Vol. 104 (Materials Research Society, Pittsburgh, Pennsylvania, 1988), p. 253.
6. "Hydrogen diffusion and passivation of shallow impurities in crystalline silicon", C. G. Van de Walle, P. J. H. Denteneer, Y. Bar-Yam, and S. T. Pantelides, in *Proceedings of the Third International Conference on Shallow Impurities in Semiconductors*, Linköping, 1988, edited by B. Monemar, IOP Conf. Ser. no. 95 (IOP London, 1989), p. 405.
7. "Diffusion of shallow impurities in silicon", C. S. Nichols, C. G. Van de Walle, and S. T. Pantelides, in *Proceedings of the Third International Conference on Shallow Impurities in Semiconductors*, Linköping, 1988, edited by B. Monemar, IOP Conf. Ser. no. 95 (IOP London, 1989), p. 493.
8. "Fluorine-silicon reactions and the etching of crystalline silicon", C. G. Van de Walle, F. R. McFeely, and S. T. Pantelides, in *Proceedings of the 19th International Conference on the Physics of Semiconductors*, Warsaw, 1988, edited by W. Zawadzki (Inst. of Physics, Polish Academy of Sciences, Warsaw, 1988), p. 789.
9. "Diffusion and complex formation in boron-doped silicon", P. J. H. Denteneer, C. S. Nichols, C. G. Van de Walle, and S. T. Pantelides, in *Proceedings of the 19th International Conference on the Physics of Semiconductors*, Warsaw, 1988, edited by W. Zawadzki (Inst. of Physics, Polish Academy of Sciences, Warsaw, 1988), p. 999.
10. "Fluorine-silicon reactions and the etching of crystalline silicon", C. G. Van de Walle, F. R. McFeely, and S. T. Pantelides, in *Proceedings of the 15th International Conference on Defects in Semiconductors*, Budapest, 1988, edited by G. Ferenczi, Mat. Sci. Forum **38-41**, 335 (Trans Tech, Aedermannsdorf, 1989).
11. "Hydrogen diffusion and passivation of shallow impurities in crystalline silicon", P. J. H. Denteneer, C. G. Van de Walle, Y. Bar-Yam, and S. T. Pantelides, in *Proceedings of the 15th International Conference on Defects in Semiconductors*, Budapest, 1988, edited by G. Ferenczi, Mat. Sci. Forum **38-41**, 979 (Trans Tech, Aedermannsdorf, 1989).

12. "Fluorine-silicon reactions and the etching of crystalline silicon", C. G. Van de Walle, F. R. McFeely, and S. T. Pantelides, in *Atomic Scale Calculations in Materials Science*, edited by J. Tersoff, D. Vanderbilt, and V. Vitek, Materials Research Society Symposia Proceedings, Vol. 141 (Materials Research Society, Pittsburgh, Pennsylvania, 1989), p. 425.
13. "Enhanced and retarded diffusion of shallow impurities in silicon", C. S. Nichols, C. G. Van de Walle, and S. T. Pantelides, in *Atomic Scale Calculations in Materials Science*, edited by J. Tersoff, D. Vanderbilt, and V. Vitek, Materials Research Society Symposia Proceedings, Vol. 141 (Materials Research Society, Pittsburgh, Pennsylvania, 1989), p. 243.
14. "Electronic structure and hyperfine parameters for hydrogen and muonium in silicon", C. G. Van de Walle, in *Impurities, Defects, and Diffusion in Semiconductors*, edited by J. Bernholc, E. E. Haller, and D. J. Wolford, Materials Research Society Symposia Proceedings, Vol. 163 (Materials Research Society, Pittsburgh, Pennsylvania, 1990), p. 419.
15. "Atomic structure of CaSi₂/Si interfaces", C. G. Van de Walle, in *Atomic Scale Structure of Interfaces*, edited by R. D. Bringans, R. M. Feenstra, and J. M. Gibson, Materials Research Society Symposia Proceedings, Vol. 159 (Materials Research Society, Pittsburgh, Pennsylvania, 1990) p. 115.
16. "Structure and hyperfine parameters of point defects in semiconductors", C. G. Van de Walle and D. B. Laks, in *Proceedings of the 20th International Conference on the Physics of Semiconductors*, Thessaloniki, 1990, edited by E. Anastassakis and J. D. Joannopoulos (World Scientific Publishing Co Pte Ltd., Singapore), p. 722.
17. "Li and native defects in ZnSe investigated by first-principles total-energy calculations", D. B. Laks, C. G. Van de Walle, G. F. Neumark, and S. T. Pantelides, in *Proceedings of the 20th International Conference on the Physics of Semiconductors*, Thessaloniki, 1990, edited by E. Anastassakis and J. D. Joannopoulos (World Scientific Publishing Co Pte Ltd., Singapore), p. 654.
18. "First-principles calculations of diffusion constants in silicon", P. E. Blöchl, C. G. Van de Walle, and S. T. Pantelides, in *Proceedings of the Second International Symposium on Process Physics and Modeling in Semiconductor Technology*, Montreal, 1990, edited by G. R. Srinivasan, J. D. Plummer, and S. T. Pantelides, (The Electrochemical Society, Inc., Pennington, NJ), p. 190.
19. "Native defect compensation in wide-band-gap semiconductors", D. B. Laks, C. G. Van de Walle, G. F. Neumark, and S. T. Pantelides, in *Proceedings of the 16th International Conference on Defects in Semiconductors*, Lehigh University, Pennsylvania, 1991, edited by G. Davies, G. G. DeLeo, and M. Stavola, *Mat. Sci. Forum* **83-87**, 1225 (Trans Tech, Zürich, 1991).

20. "First-principles investigations of acceptors in ZnSe", C. G. Van de Walle and D. B. Laks, in *Wide Band-Gap Semiconductors*, edited by T. D. Moustakas, J. I. Pankove, and Y. Hamakawa, Materials Research Society Symposia Proceedings, Vol. 242 (Materials Research Society, Pittsburgh, Pennsylvania, 1992), p. 349.
21. "Self-compensation and doping problems in ZnSe", D. B. Laks and C. G. Van de Walle, in *Wide Band-Gap Semiconductors*, edited by T. D. Moustakas, J. I. Pankove, and Y. Hamakawa, Materials Research Society Symposia Proceedings, Vol. 242 (Materials Research Society, Pittsburgh, Pennsylvania, 1992), p. 311.
22. "First-principles investigations of hydrogen and fluorine on silicon surfaces", C. G. Van de Walle, in *Chemical Surface Preparation, Passivation and Cleaning for Semiconductor Growth and Processing*, edited by R. J. Nemanich, C. R. Helms, M. Hirose, and G. W. Rubloff, Materials Research Society Symposia Proceedings, Vol. 259 (Materials Research Society, Pittsburgh, Pennsylvania), p. 375.
23. "First-principles investigations of hydrogen, oxygen, and fluorine interactions with silicon", C. G. Van de Walle, in *Proceedings of the Third International Symposium on Process Physics and Modeling in Semiconductor Technology*, edited by G. R. Srinivasan, K. Taniguchi, and C. S. Murthy, Volume 93-6 (The Electrochemical Society, Pennington, NJ, 1993), p. 429-442.
24. "Native defects and impurities in cubic and wurtzite GaN", J. Neugebauer and C. G. Van de Walle, in *Diamond, SiC and Nitride Wide Bandgap Semiconductors*, edited by C. H. Carter Jr., G. Gildenblat, S. Nakamura, and R. J. Nemanich, Materials Research Society Symposia Proceedings, Vol. 339 (Materials Research Society, Pittsburgh, Pennsylvania, 1994), p. 687.
25. "Defects and doping in GaN", J. Neugebauer and C. G. Van de Walle, in *Proceedings of the 22th International Conference on the Physics of Semiconductors*, Vancouver, 1994, edited by D. J. Lockwood (World Scientific Publishing Co Pte Ltd., Singapore), p. 2327.
26. "Isolated hydrogen in silicon – a large negative-U system", N. M. Johnson, C. Herring, and C. G. Van de Walle, in *Proceedings of the 22th International Conference on the Physics of Semiconductors*, Vancouver, 1994, edited by D. J. Lockwood (World Scientific Publishing Co Pte Ltd., Singapore), p. 2227.
27. "Hydrogen Interactions with Crystalline, Amorphous, Polycrystalline, and Porous Silicon", C. G. Van de Walle, in *Proceedings of the CAM-94 Physics Meeting (Joint Meeting of the Canadian Association of Physicists, the American Physical Society, and the Mexican Physical Society)*, edited by A. Zepeda, AIP Conference Proceedings Series, Vol. 342 (AIP Press, Woodbury, New York, 1995), p. 15.
28. "Atomic hydrogen in GaN", J. Neugebauer and C. G. Van de Walle, in *Defect and Impurity Engineered Semiconductors and Devices*, edited by S. Ashok, I. Akasaki, J. Chevallier, and N. M. Johnson, Materials Research Society Symposia Proceedings, Vol. 378 (Materials Research Society, Pittsburgh, Pennsylvania, 1995), p. 503.

29. "Phase stability and electronic structure of GaAs_{1-x}N_x alloys", J. Neugebauer and C. G. Van de Walle, in *Strained Layer Epitaxy – Materials, Processing, and Device Applications*, edited by E. Fitzgerald, K.-Y. Cheng, J. Hoyt, and J. Bean, Materials Research Society Symposia Proceedings, Vol. 379 (Materials Research Society, Pittsburgh, Pennsylvania, 1995), p. 3.
30. "Theory of defects in wide-band-gap semiconductors", C. G. Van de Walle and J. Neugebauer, in *Defect and Impurity Engineered Semiconductors and Devices*, edited by S. Ashok, I. Akasaki, J. Chevallier, and N. M. Johnson, Materials Research Society Symposia Proceedings, Vol. 378 (Materials Research Society, Pittsburgh, Pennsylvania, 1995), p. 467.
31. "Silicon-hydrogen bonding and hydrogen diffusion in amorphous silicon", C. G. Van de Walle and R. A. Street, in *Amorphous Silicon Technology*, edited by E. A. Schiff, M. Hack, A. Madan, and A. Matsuda, Materials Research Society Symposia Proceedings, Vol. 377 (Materials Research Society, Pittsburgh, Pennsylvania, 1995), p. 389.
32. "Theory of point defects and complexes in GaN", J. Neugebauer and C. G. Van de Walle, in *Gallium Nitride and Related Materials*, edited by R. D. Dupuis, J. A. Edmond, F. A. Ponce, and S. Nakamura, Materials Research Society Symposia Proceedings, Vol. 395 (Materials Research Society, Pittsburgh, Pennsylvania), p. 645.
33. "Tight-binding initialization for generating high-quality initial wave functions: application to defects and impurities in GaN", J. Neugebauer and C. G. Van de Walle, in *Materials Theory, Simulations, and Parallel Algorithms*, edited by E. Kaxiras, J. Joannopoulos, P. Vashishta, and R. K. Kalia, Materials Research Society Symposia Proceedings, Vol. 408 (Materials Research Society, Pittsburgh, Pennsylvania), p. 43.
34. "Hydrogen in GaN", N. M. Johnson, W. Götz, J. Neugebauer and C. G. Van de Walle, in *Gallium Nitride and Related Materials*, edited by R. D. Dupuis, J. A. Edmond, F. A. Ponce, and S. Nakamura, Materials Research Society Symposia Proceedings, Vol. 395 (Materials Research Society, Pittsburgh, Pennsylvania, 1996), p. 723.
35. "Hydrogen diffusion and complex formation in GaN", J. Neugebauer, W. Götz, and C. G. Van de Walle, in *Proceedings of the 6th International Conference on SiC and Related Materials*, Kyoto, Japan, Sept. 18-21, 1995, edited by S. Nakashima, H. Matsunami, S. Yoshida, and H. Harima, Inst. Phys. Conf. Ser. No 142 (IOP Publishing, Bristol, 1996), p. 1035.
36. "New model for "stretched exponential" relaxation", C. G. Van de Walle, in *Amorphous Silicon Technology*, edited by M. Hack, R. Schropp, E. A. Schiff, A. Matsuda, and S. Wagner, Materials Research Society Symposia Proceedings, Vol. 420 (Materials Research Society, Pittsburgh, Pennsylvania, 1996), p. 533.

37. "Role of hydrogen and hydrogen complexes in doping of GaN", J. Neugebauer and C. G. Van de Walle, in *III-Nitride, SiC, and Diamond Materials for Electronic Devices*, edited by D. K. Gaskill, C. Brandt, and R. J. Nemanich, Materials Research Society Symposia Proceedings, Vol. 423 (Materials Research Society, Pittsburgh, Pennsylvania, 1996), p. 619.
38. "Role of defects and impurities in doping of GaN", J. Neugebauer and C. G. Van de Walle, in *Proceedings of the 23rd International Conference on the Physics of Semiconductors*, Berlin, 1996, edited by M. Scheffler and R. Zimmermann (World Scientific Publishing Co Pte Ltd., Singapore, 1996), p. 2849.
39. "Theory of point defects and interfaces", C. G. Van de Walle and J. Neugebauer, in *III-V Nitrides*, edited by F. A. Ponce, T. D. Moustakas, I. Akasaki, and B. A. Monemar, Materials Research Society Symposia Proceedings, Vol. 449 (Materials Research Society, Pittsburgh, Pennsylvania, 1997), p. 861.
40. "Defects and doping in III-V nitrides", C. G. Van de Walle and J. Neugebauer, in *Proceedings of the 19th International Conference on Defects in Semiconductors*, Aveiro, Portugal, 1997, edited by G. Davies and M. H. Nazaré, Mat. Sci. Forum **258-263**, (Trans Tech, Zürich, 1997), p. 19.
41. "Theoretical study of native point defects in AlN and InN", C. Stampfl and C. G. Van de Walle, in *Nitride Semiconductors*, edited by F. A. Ponce, S. P. DenBaars, B. K. Meyer, S. Nakamura, and S. Strite, Materials Research Society Symposia Proceedings, Vol. 482 (Materials Research Society, Pittsburgh, Pennsylvania, 1998), p. 905.
42. "Defects, doping and interfaces in III-V nitrides", C. G. Van de Walle, in *Physics and Simulation of Optoelectronic Devices VI*, edited by M. Osinski, P. Blood, and A. Ishibashi, SPIE Proc. Volume 3283 (SPIE, Bellingham, 1998), p. 52.
43. "Theory of hydrogen in semiconductors", C. G. Van de Walle, in *Hydrogen in Semiconductors and Metals*, edited by R. C. Bowman, W. B. Jackson, R. G. Leisure, and N. H. Nickel, MRS Symposia Proceedings, Vol. 513 (MRS, Pittsburgh, Pennsylvania, 1998), p. 55.
44. "Evidence for oxygen DX centers in AlGaIn", M. D. McCluskey, N. M. Johnson, C. G. Van de Walle, D. P. Bour, M. Kneissl, and W. Walukiewicz, in *Wide-Bandgap Semiconductors for High Power, High Frequency and High Temperature*, edited by S. DenBaars, J. Palmour, M. Shur, and M. Spencer, Materials Research Society Symposia Proceedings, Vol. 512 (MRS, Pittsburgh, Pennsylvania, 1998), p. 531.
45. "Doping of AlGaIn alloys", C. G. Van de Walle, C. Stampfl, J. Neugebauer, M. D. McCluskey, and N. M. Johnson, *GaN and Related Alloys*, edited by C. R. Abernathy and B. Monemar, Materials Research Society Symposia Proceedings, Vol. **537** (Materials Research Society, Pittsburgh, Pennsylvania, 1998); MRS Internet J. Nitride Semicond. Res. **4S1**, G10.4 (1999).

46. "Theory of hydrogen interactions with amorphous silicon", C. G. Van de Walle and B. Tuttle, in *Amorphous and Heterogeneous Silicon Thin Films -- Fundamentals to Devices*, edited by H. M. Branz, R. W. Collins, H. Okamoto, S. Guha, and R. Schropp, MRS Symposia Proceedings, Vol. **557** (MRS, Pittsburgh, Pennsylvania, 1999), p. 275.
47. "New insights in doping of III-nitrides and their alloys", C. G. Van de Walle and J. Neugebauer, in *Proceedings of the 26th International Symposium on Compound Semiconductors*, edited by K. H. Ploog, G. Tränkle, and G. Weimann, Inst. Phys. Conf. Ser. No. **166**, p. 439 (2000).
48. "Theory of impurities and defects in III-nitrides: Vacancies in GaN and related materials", C. G. Van de Walle, in *Proceedings of the International Conference on Silicon Carbide and Related Materials*, Raleigh, North Carolina, 1999, edited by C. H. Carter, Jr., R. P. Devaty, and G. S. Rohrer, Mat. Sci. Forum **338-342** (Trans Tech, Zürich, 2000), p. 1561.
49. "Controlling the conductivity of wide-band-gap semiconductors", C. G. Van de Walle and J. Neugebauer, in *Proceedings of the 25th International Conference on the Physics of Semiconductors*, Osaka, 2000, edited by N. Miura and T. Ando (Springer, Berlin, 2001), p. 3.
50. "Stability, diffusion, and complex formation of beryllium in wurtzite GaN", S. Limpijumnong, C. G. Van de Walle, and J. Neugebauer, in *GaN and Related Alloys*, edited by U. Mishra, M. S. Shur, C. M. Wetzel, B. Gil, and K. Kishino, Materials Research Society Symposium Proceedings, Vol. **639**, G4.3 (2001).
51. "Performance characteristics of cw InGaN multiple-quantum-well laser diodes", M. Kneissl, W. S. Wong, C. G. Van de Walle, J. E. Northrup, D. W. Treat, M. Teepe, N. Miyashita, P. Kiesel, and N. M. Johnson, in *GaN and Related Alloys*, edited by U. Mishra, M. S. Shur, C. M. Wetzel, B. Gil, and K. Kishino, Materials Research Society Symposium Proceedings, Vol. **639**, G10.6 (2001).
52. "Vibrational spectroscopy of GaN:Mg under pressure", M. D. McCluskey, K. K. Zhuravlev, M. Kneissl, W. Wong, D. Treat, S. Limpijumnong, C. G. Van de Walle, and N. M. Johnson, in *GaN and Related Alloys*, edited by J. E. Northrup, J. Neugebauer, S. F. Chichibu, D. C. Look, and H. Riechert, Materials Research Society Symposium Proceedings, Vol. **693**, I2.4 (2002).
53. "Novel configuration of Mg-H complexes in GaN", S. Limpijumnong, J. E. Northrup, and C. G. Van de Walle, in *GaN and Related Alloys*, edited by J. E. Northrup, J. Neugebauer, S. F. Chichibu, D. C. Look, and H. Riechert, Materials Research Society Symposium Proceedings, Vol. **693**, I2.5 (2002).
54. "Effects of stoichiometry on point defects and impurities in gallium nitride", C. G. Van de Walle, J. E. Northrup, and J. Neugebauer, in *Proceedings of the 4th Symposium on Non-Stoichiometric III-V Compounds*, Asilomar, CA, October 2-4, 2002, edited by P. Specht, T. R. Weatherford, P. Kiesel, T. Marek, and S. Malzer (Friedrich-Alexander-Universität, Erlangen-Nürnberg 2002), p. 11.

55. "Hydrogen interactions with semiconductors and oxides", C. G. Van de Walle, in *Proceedings of the International Workshop on Hydrogen in Materials and Vacuum Systems*, Jefferson Lab, Newport News, Virginia, November 11-13, 2002, edited by G. R. Myneni and S. Chattopadhyay, AIP Conference Proceedings Vol. **671** (Melville, New York, 2003), p. 33.
56. "Direct determination of the built-in polarization field in InGaN/GaN quantum wells", R. Schmidt, P. Kiesel, M. Kneissl, C. G. Van de Walle, N.M. Johnson, F. Renner, and G. H. Döhler, in *Proceedings of SIMC-XII-2002 (Semiconducting and Insulating Materials Conference)*, IEEE Catalog Number: 02CH37343 (ISBN: 0-7803-7418-5), 48-51 (2003).
57. "Effects of ionicity on defect physics of wide-band-gap semiconductors", C. G. Van de Walle, in *Proceedings of the International Conference on Silicon Carbide and Related Materials*, Lyon, France, October 5-10, 2003, edited by R. Madar, J. Camassel and E. Blanquet, Mater. Sci. Forum **457-460**, pp. 15-20 (2004).
58. "Theory of hydrogen-related levels in semiconductors and oxides", C. G. Van de Walle, IEEE International Electron Devices Meeting (IEDM) Technical Digest, 2005, p. 400.
59. "Properties of ZnO(0001) layers grown by metalorganic chemical vapor deposition on GaN(0001) templates", T. Ive, T. Ben-Yaacov, H. Asamizu, C. G. Van de Walle, U. Mishra, S. P. DenBaars, and J. S. Speck, phys. stat. sol. (c) **5**, 1733 (2008).
60. "Metalorganic chemical vapor deposition of ZnO(0001) thin films on GaN(0001) templates and ZnO(0001) substrates", T. Ive, T. Ben-Yaacov, A. Murai, H. Asamizu, C. G. Van de Walle, U. Mishra, S. P. DenBaars, and J. S. Speck, phys. stat. sol. (c) **5**, 3091 (2008).
61. "Technology development & design for 22 nm InGaAs/InP-channel MOSFETs", M. Rodwell, M. Wistey, U. Singiseti, G. Burek, A. Gossard, S. Stemmer, R. Engel-Herbert, Y. Hwang, Y. Zheng, C. Van de Walle, P. Asbeck, Y. Taur, A. Kummel, B. Yu, D. Wang, Y. Yuan, C. Palmstrom, E. Arkun, P. Simmonds, P. McIntyre, J. Harris, M. V. Fischetti, and C. Sachs, in *Proceedings of the 2008 IEEE 20th International Conference on Indium Phosphide & Related Materials (IPRM)* (2008); doi: 10.1109/ICIPRM.2008.4703065.
62. "Hydrogen in oxides and nitrides: unexpected physics and impact on devices", C. G. Van de Walle and A. Janotti, in *Proceedings of the 11th Europhysical Conference on Defects in Insulating Materials (EURODIM 2010)* (IOP Publishing), IOP Conf. Series: Mater. Sci. Eng. **15**, 012001 (2010). [doi:10.1088/1757-899X/15/1/012001]
63. "Vacancy defects in indium oxide: An ab-initio study", P. Reunchan, X. Zhou, S. Limpijumnong, A. Janotti, and C. G. Van de Walle, Current Appl. Phys. **11**, S296 (2011). [doi: 10.1016/j.cap.2011.03.051]

64. “Conductivity and transparency of TiO₂ from first principles”, A. Schleife, J. B. Varley, A. Janotti, and C. G. Van de Walle, in *Solar Hydrogen and Nanotechnology VIII*, edited by Y. Kanai and D. Prendergast, Proc. of SPIE Vol. 8822, 882205 (2013). [doi: [10.1117/12.2024566](https://doi.org/10.1117/12.2024566)]
65. “Auger recombination in light-emitting materials”, E. Kiopakis, Q. Yan, and C. G. Van de Walle, in CLEO: 2014, OSA Technical Digest (online) (Optical Society of America, 2014), paper SM1J.5.
66. “Auger recombination in InAs: Role of spin-orbit coupling and phonons”, J.-X. Shen, D. Steiauf, E. Kiopakis, and C. G. Van de Walle, Proceedings of the 2016 Compound Semiconductor Week (CSW), IEEE (2016). [[10.1109/ICIPRM.2016.7528804](https://doi.org/10.1109/ICIPRM.2016.7528804)]
67. “First-principles characterization of defects in WO₃”, W. Wang, H. Peelaers, J.-X. Shen, A. Janotti, and C. G. Van de Walle, in *Oxide-based Materials and Devices IX*, edited by D. J. Rogers, D. C. Look, and F. H. Teherani, Proc. SPIE 10533, 105332C (2018). [doi: [10.1117/12.2303688](https://doi.org/10.1117/12.2303688)]
68. “First-principles calculations of optical transitions at native defects and impurities in ZnO”, J. L. Lyons, J. B. Varley, A. Janotti, and C. G. Van de Walle, in *Oxide-based Materials and Devices IX*, edited by D. J. Rogers, D. C. Look, and F. H. Teherani, Proc. SPIE 10533, 105331O (2018). [doi: [10.1117/12.2303687](https://doi.org/10.1117/12.2303687)]

PATENTS

1. "TM-polarized laser emitter using III-V alloy with nitrogen", C. G. Van de Walle and D. P. Bour, U. S. Patent No. 5,383,211 (1995).
2. "Dual polarization quantum well laser in the 200 to 600 nanometers range", C. G. Van de Walle, U. S. Patent No. 5,828,684 (1998).
3. "Optoelectronic devices based on ZnGeN₂ integrated with group III-V nitrides", C. G. Van de Walle, U.S. Patent No. 6,121,639 (2000).
4. "Light-emitting devices including polycrystalline GaN layers and method of forming devices", N. H. Nickel, C. G. Van de Walle, D. P. Bour, and P. Mei, U.S. Patent Number 6,288,417 (2001).
5. "Structure and method for asymmetric waveguide nitride laser diode", C. G. Van de Walle, D. P. Bour, M. A. Kneissl, and L. T. Romano, U.S. Patent Number 6,389,051 (2002).
6. "Structure and method for asymmetric waveguide nitride laser diode", C. G. Van de Walle, D. P. Bour, M. A. Kneissl, and L. T. Romano, U.S. Patent Number 6,430,202 (8/602).
7. "Semiconductor device and method of forming a semiconductor device", J. E. Northrup and C. G. Van de Walle, U.S. Patent Number 6,437,374 (2002).
8. "Nitride-based VCSEL or light emitting diode with p-n tunnel junction current injection", M. Kneissl, P. Kiesel, and C. G. Van de Walle, U.S. Patent Number 6,515,308 (2/4/03).
9. "Method for forming an asymmetric nitride laser diode", C. G. Van de Walle, D. P. Bour, M. A. Kneissl, and L. T. Romano, U.S. Patent Number 6,541,292 B2 (4/1/03).
10. "Structure and method for self-aligned, index-guided, buried heterostructure AlGaInN laser diodes", D. Bour, M. Kneissl, L. Romano, T. L. Paoli, and C. G. Van de Walle, U.S. Patent Number 6,567,443 (5/20/03).
11. "Structure and method for index-guided buried heterostructure AlGaInN laser diodes", D. Bour, M. Kneissl, L. Romano, T. L. Paoli, and C. G. Van de Walle, U.S. Patent Number 6,570,898 (5/27/03).
12. "Distributed feedback laser fabricated by lateral overgrowth of an active region", D. Hofstetter, T. L. Paoli, L. T. Romano, D. Sun, D. P. Bour, M. A. Kneissl, C. G. Van de Walle, and N. M. Johnson, U.S. Patent Number 6,574,256 (2003).
13. "Semiconductor device and method of forming a semiconductor device", J. E. Northrup and C. G. Van de Walle, U.S. Patent Number 6,583,449 (6/24/03).
14. "Semiconductor structures having reduced contact resistance", C. G. Van de Walle, U.S. Patent Number 6,605,832 (8/12/03).

15. "Edge-emitting nitride-based laser diode with p-n tunnel junction current injection", M. Kneissl, P. Kiesel, and C. G. Van de Walle, U.S. Patent Number 6,724,013 (4/20/04).
16. "Laser Diode with metal-oxide upper cladding layer", M. A. Kneissl, L. T. Romano, and C. G. Van de Walle, U.S. Patent Number 6,990,132 (1/24/2006).
17. "Nitride-based laser diode with GaN waveguide/cladding layer", M. A. Kneissl, D. P. Bour, L. T. Romano, and C. G. Van de Walle, U.S. Patent Number 7,123,637 (10/17/2006).
18. "Systems and methods for electrical contacts to arrays of vertically aligned nanorods", T. Hantschel, N. M. Johnson, P. Kiesel, C. G. Van De Walle, and W. S. Wong, U.S. Patent Number 7,202,173 (4/10/2007).
19. "Surface-passivated zinc-oxide based sensor", C. G. Van de Walle, P. Kiesel, and O. Schmidt, U.S. Patent Number 7,432,526 (B2) (10/7/2008).
20. "Micro-machined fuel cells", R. B. Apte, D. G. Duff, C. G. Van de Walle, J. P. Lu, A. Salleo, and S. D. White, U.S. Patent Number 7,459,225 (12/2/2008).
21. "Systems and methods for electrical contacts to arrays of vertically aligned nanorods", T. Hantschel, N. M. Johnson, P. Kiesel, C. G. Van de Walle, and W. S. Wong, U.S. Patent Number 7,569,905 (8/4/2009).
22. "Method for surfaced-passivated zinc-oxide", C. G. Van de Walle, P. Kiesel, and O. Schmidt, U.S. Patent Number 7,745,272; (6/29/2010).
23. "Micro-machined fuel cells", R. B. Apte, D. G. Duff, C. G. Van de Walle, J. P. Lu, A. Salleo, and S. D. White, U.S. Patent Number 7,811,692; (10/12/2010).
24. "Systems and methods for electrical contacts to arrays of vertically aligned nanorods", T. Hantschel, N. M. Johnson, P. Kiesel, C. G. Van de Walle, and W. S. Wong, U.S. Patent Number 8,617,407 (12/31/2013).

Several patents pending.

INVITED CONFERENCE PRESENTATIONS

Chris G. Van de Walle

1. "Hydrogen in crystalline silicon", Sixth International Conference on Deep Impurity Levels, Santa Margherita di Pula, Sardinia, Italy, September 22-25, 1987.
2. "Hydrogen diffusion and reactions in crystalline silicon", Workshop on Computational Condensed Matter Physics, Glion-sur-Montreux, Switzerland, February 24-26, 1988.
3. "Theory of hydrogen diffusion and reactions in crystalline silicon", March Meeting of the American Physical Society, New Orleans, Louisiana, March 21-25, 1988.
4. "Physics of heterojunctions", IMEC Summer Course on Physics of Advanced Microdevices, Leuven, Belgium, June 13-16, 1988.
5. "The model solid theory for heterojunction band offsets", CECAM Workshop on Calculation of Electronic, Structural, and Lattice-Dynamical Properties of Semiconductor Interfaces and Superlattices, CECAM, Université Paris - Sud, France, June 20-July 1, 1988.
6. "Hydrogen diffusion and passivation of shallow impurities in crystalline silicon", Third International Conference on Shallow Impurities in Semiconductors, Linköping, Sweden, August 10-12, 1988.
7. "Theory of hydrogen diffusion and reactions in crystalline semiconductors", Workshop on Hydrogen Passivation of Dopants and Defects in III-V Compounds and their Alloys, Universités Pierre & Marie Curie and Paris 7, Paris, France, Nov. 3-4, 1988.
8. "Fluorine-silicon reactions and the etching of crystalline silicon", Fall Meeting of the Materials Research Society, Boston, Massachusetts, November 28-December 3, 1988.
9. "Theoretical aspects of hydrogen in crystalline semiconductors", Sixth Trieste Semiconductor Symposium: Hydrogen in Semiconductors, International Center for Theoretical Physics, Trieste, Italy, August 27-31, 1990.
10. "Structure and energy of interstitial hydrogen and hydrogen-related complexes in crystalline semiconductors", Workshop on Hydrogen Migration and the Stability of Hydrogen Related Complexes in Crystalline Semiconductors, Freiburg, Germany, November 3-6, 1991.
11. "First-principles investigations of hydrogen and fluorine on silicon surfaces", Spring Meeting of the Materials Research Society, San Francisco, California, April 27-May 1, 1992.
12. "Solubility, defect reactions, and doping limits in ZnSe", Gordon Research Conference on Point Defects, Line Defects, and Interfaces in Semiconductors, Plymouth, NH, July 20-24, 1992.
13. **Keynote talk:** "First-principles investigations of hydrogen and fluorine interactions with silicon", First International Symposium on Ultra Clean Processing of Silicon Surfaces, Leuven, Belgium, September 17-19, 1992.

14. "First-principles calculations of light emission from Si-based materials", March Meeting of the American Physical Society, Seattle, Washington, March 22-26, 1993.
15. "First-principles investigations of hydrogen, oxygen, and fluorine interactions with silicon", Third International Symposium on Process Physics and Modeling in Semiconductor Technology, 183rd Meeting of the Electrochemical Society, Honolulu, Hawaii, May 16-21, 1993.
16. "Solubilities, compensation, and doping limits in compound semiconductors", European Research Conference on Electronic Structure of Solids, Porto Carras, Greece, September 18-23, 1993.
17. "Nitrogen doping in ZnTe and ZnSe", Sixth International Conference on Shallow Level Centers in Semiconductors, Berkeley, CA, August 10-12, 1994.
18. "Defects, impurities, and doping levels in semiconductors", 5th Italian-Swiss Workshop on Computational Condensed Matter Physics, Santa Margherita di Pula, Sardinia, Italy, September 8-13, 1994.
19. "Hydrogen Interactions with Crystalline, Amorphous, Polycrystalline, and Porous Silicon", CAM 94: Joint Meeting of the Canadian Association of Physicists, the American Physical Society, and the Mexican Physical Society, Cancun, Mexico, September 26-30, 1994.
20. "Theory of defects in wide-band-gap semiconductors", Spring Meeting of the Materials Research Society, San Francisco, California, April 17-21, 1995.
21. "Theory of defects in semiconductors", Fifth Conference on Computational Research on Materials, Morgantown, West Virginia, May 3-5, 1995.
22. "Theory of doping in wide-band-gap semiconductors", Fifth International Conference on the Formation of Semiconductor Interfaces, Princeton University, New Jersey, June 26-30, 1995.
23. "Defects, impurities and doping in GaN", March Meeting of the American Physical Society, St. Louis, Missouri, March 18-22, 1996.
24. "Defects, impurities, and doping in gallium nitride", Spring Meeting of the Materials Research Society, San Francisco, California, April 8-12, 1996.
25. "Hydrogen in GaN: Novel aspects of a common impurity", 160. WE-Heraeus Seminar: Hydrogen in Solids and at Solid Surfaces, Ilmenau, Germany, May 30-June 1, 1996.
26. "Theory of point defects and interfaces", Fall Meeting of the Materials Research Society, Boston, Massachusetts, December 2-6, 1996.
27. "Defects and doping in GaN", 8th Brazilian Workshop on Semiconductor Physics, São Paulo, Brazil, February 2-7, 1997.
28. **Plenary talk:** "Defects and doping in III-V nitrides", 19th International Conference on Defects in Semiconductors, Aveiro, Portugal, July 21-25, 1997.

29. "Hydrogen states in silicon", 17th International Conference on Amorphous and Microcrystalline Semiconductors, Budapest, Hungary, August 25-29, 1997.
30. "Hydrogen in silicon: fundamental properties and consequences for devices", 44th National Symposium of the American Vacuum Society, San Jose, California, October 20-24, 1997.
31. "Theory of doping and defects in III-V nitrides", Second International Conference on Nitride Semiconductors, Tokushima, Japan, October 27-31, 1997.
32. "Interfaces and band offsets in III-nitrides", International GaN Workshop, Schloss Ringberg, Rottach-Egern, Germany, January 20-24, 1998
33. "Defects, doping and interfaces in III-V nitrides", Photonics West Optoelectronics '98, San Jose, California, January 24-30, 1998.
34. "Blue lasers: materials growth, characterization, and computational physics", Workshop on "Science and Mathematical Science: Exploring the Interface", National Research Council, Washington, DC, March 25-26, 1998.
35. "Theory of hydrogen in semiconductors", Spring Meeting of the Materials Research Society, San Francisco, California, April 12-17, 1998.
36. "First-principles calculations of energetics and dissociation of Si-H bonds", Workshop on the Role of Hydrogen and Deuterium in Hot Electron Semiconductor Device Degradation, Urbana, Illinois, April 20-21, 1998.
37. "Energetics and vibrational frequencies of interstitial H₂ molecules in semiconductors", Spring Meeting of the European Materials Research Society, Strasbourg, France, June 16-19, 1998.
38. "III-V nitrides: successes and challenges", Deutsche Forschungsgemeinschaft Colloquium on "Group III Nitrides and their Heterostructures", Bad Honnef, Germany, October 26-27, 1998.
39. "Doping of AlGaIn alloys", Fall Meeting of the Materials Research Society, Boston, Massachusetts, November 30 - December 4, 1998.
40. "Theory of hydrogen interactions with amorphous silicon", Spring Meeting of the Materials Research Society, San Francisco, California, April 5-9, 1999.
41. "Interactions of hydrogen with silicon and consequences for devices", Workshop on Hydrogen in Semiconductors, Exeter, England, April 15-16, 1999.
42. "Defects and Defect Reactions in Semiconductor Nitrides", XXVIII International School on Physics of Semiconducting Compounds, Jaszowiec, Poland, June 7-11, 1999.
43. "Effect of native point defects on nitride materials and devices", Electronic Materials Conference, Santa Barbara, California, June 30-July 2, 1999.

44. “New insights in doping of III-nitrides and their alloys”, International Symposium on Compound Semiconductors, Berlin, Germany, August 22-26, 1999.
45. “Theory of impurities and defects in III-nitrides”, International Conference on Silicon Carbide and Related Materials, Raleigh, North Carolina, October 10-15, 1999.
46. “First-principles calculations of defects and impurities in GaN, AlN, and InN”, Workshop on “Advances in First-Principles Computational Condensed Matter Physics”, Miraflores de la Sierra (Madrid), Spain, January 13-15, 2000.
47. “First-principles studies of defects and impurities in nitride semiconductors”, “Fifteen Years of the Car-Parrinello Method in Physics and Chemistry”, Minneapolis, Minnesota, March 18-19, 2000.
48. “Hydrogen diffusion and metastability in hydrogenated amorphous silicon”, CECAM Workshop on Electronic and Optical Properties of Semiconducting Glasses, Lyon, France, June 13-16, 2000.
49. “Sources of n-type conductivity in ZnO”, Gordon Research Conference on Point & Line Defects in Semiconductors, Colby-Sawyer College, New London, NH, July 9-14, 2000.
50. “Properties of GaN surfaces: the role of hydrogen”, \square 2000 Conference: “Ab initio calculations of complex processes in materials”, Schwäbisch Gmünd, Germany, August 22-26, 2000.
51. **Plenary talk:** “Controlling the conductivity of wide-band-gap semiconductors”, 25th International Conference on the Physics of Semiconductors, Osaka, Japan, September 17-22, 2000.
52. “Role of hydrogen in surface reconstructions and growth of GaN”, Fall Meeting of the Materials Research Society, Boston, Massachusetts, November 26 - December 1, 2000.
53. “Hydrogen as a cause of doping in ZnO”, March Meeting of the American Physical Society, Seattle, Washington, March 12-16, 2001.
54. “Dopant engineering in wide-band-gap semiconductors”, WideGap 2001: Doping Issues in Wide-Band-Gap Semiconductors, Exeter, England, March 21-23, 2001.
55. “Defect analysis and engineering in ZnO”, 21st International Conference on Defects in Semiconductors, Giessen, Germany, July 16-20, 2001.
56. “Strategies for controlling the conductivity of wide-band-gap semiconductors”, 10th International Conference on II-VI Compounds, Bremen, Germany, September 9-14, 2001.
57. “Role of hydrogen in surface reconstructions and growth of GaN”, 29th International Conference on Physics in Semiconductors, Santa Fe, New Mexico, January 6-10, 2002.
58. **Adler Award Lecture:** “The fascinating physics of hydrogen in semiconductors and oxides”, March Meeting of the American Physical Society, Indianapolis, Indiana, March 18-22, 2002.

59. "Defect and Impurity Engineering in ZnO", Spring Meeting of the Materials Research Society, San Francisco, California, April 1-5, 2002.
60. "Defects and doping in wide-band-gap semiconductors", 19th General Conference of the Condensed Matter Division of the European Physical Society, Brighton, United Kingdom, April 7-11, 2002.
61. "Structure and energetics of nitride surfaces under MOCVD growth conditions", 11th International Conference on Metal-Organic Vapour Phase Epitaxy, Berlin, Germany, June 3-7, 2002.
62. "Hydrogen as a shallow center in semiconductors and oxides", 10th International Conference on Shallow Level Centers in Semiconductors, Warsaw, Poland, July 24-27, 2002.
63. "Materials and device design of nitride-based blue lasers", Second International Conference on Numerical Simulation of Optoelectronic Devices, Zürich, Switzerland, September 25-27, 2002.
64. "Effects of stoichiometry on point defects and impurities in GaN", Fourth Symposium on Non-Stoichiometric III-V Compounds, Asilomar, California, October 2-4, 2002.
65. "Hydrogen as a shallow center in semiconductors and oxides", International Workshop on Hydrogen in Materials and Vacuum Systems, Newport News, Virginia, November 11-13, 2002.
66. "Effects of hydrogen in devices", Twenty-Five Years of Ultra-Small Electronics Research, Hapuna Beach, Hawaii, November 29, 2002.
67. "Structure and energetics of nitride surfaces under realistic growth conditions", March Meeting of the American Physical Society, Austin, Texas, March 3-7, 2003.
68. "Role of hydrogen in doping of wide-band-gap semiconductors", First NIMS (National Institute for Materials Science) International Conference: Materials Solutions for Photonics, Tsukuba, Japan, March 17-19, 2003.
69. **Plenary talk:** "Effects of ionicity on defect physics of wide-band-gap semiconductors", International Conference on Silicon Carbide and Related Materials, Lyon, France, October 5-10, 2003.
70. "Electronic materials theory: Interfaces and defects", 50th Anniversary Session, AVS 50th International Symposium, Baltimore, Maryland, November 2-7, 2003.
71. "Effects of hydrogen on electronic properties of low-band-gap semiconductors", Fall Meeting of the Materials Research Society, Boston, Massachusetts, December 1-5, 2003.
72. "New applications of ZnO in electronics and optoelectronics", Materials Research Outreach Symposium, University of California, Santa Barbara, California, January 28-30, 2004.
73. "Universal alignment of hydrogen levels in semiconductors, insulators, and solutions", Max Planck Society / UCSB Workshop on Future Trends in Materials, Santa Barbara, California, February 22-25, 2004.

74. "Hydrogen as a shallow center in semiconductors", Spring Meeting of the Materials Research Society, San Francisco, California, April 12-16, 2004.
75. "Doping and defects in AlN and InN", Spring Meeting of the European Materials Research Society, Strasbourg, France, May 25-28, 2004.
76. "Hydrogen interactions with semiconductors, oxides, and their interfaces", 35th IEEE Semiconductor Interface Specialists Conference, San Diego, California, December 9-11, 2004.
77. "Role of hydrogen in doping of oxides", 4th International Symposium on Transparent Oxide Thin Films for Electronics and Optics, Tokyo, Japan, April 7-8, 2005.
78. "New applications of ZnO in optoelectronics and electronics", Complex Functional Oxides: A joint UC/Los Alamos National Laboratories Workshop, Santa Barbara, California, May 13-14, 2005.
79. **Plenary talk:** "Universal alignment of hydrogen levels in semiconductors, insulators, and solutions", 2nd International Symposium on Hydrogen in Matter, Uppsala, Sweden, June 13-17, 2005.
80. "Universal alignment of hydrogen levels in semiconductors, insulators, and solutions", 10th International Conference on the Formation of Semiconductor Interfaces, Aix-en-Provence, France, July 3-8, 2005.
81. **Plenary talk:** "Universal alignment of hydrogen levels in semiconductors and insulators", 23rd International Conference on Defects in Semiconductors, Awaji Island, Japan, July 25-29, 2005.
82. "Oxides as semiconductors", Max Planck Society / UCSB Workshop on Future Trends in Material Sciences, Berlin, Germany, September 11-14, 2005.
83. "Defect physics and nonstoichiometry in wide-band-gap semiconductors", 2nd International Symposium on Point Defects and Nonstoichiometry, Kaohsiung, Taiwan, October 3-7, 2005.
84. "Theory of hydrogen-related levels in semiconductors and oxides", IEEE International Electron Device Meeting, Washington, DC, December 5-7, 2005.
85. "New insights in defect physics of ZnO", Materials Research Outreach Symposium, University of California, Santa Barbara, California, January 25-27, 2006.
86. "Theory of defects and doping in ZnO", March Meeting of the American Physical Society, Baltimore, Maryland, March 13-17, 2006.
87. "Electronic structure of nitride surfaces", First International Symposium on Growth of III-Nitrides", Linköping, Sweden, June 4-7, 2006.
88. "Defects and doping in ZnO", ZnO-Rundgespräch, Deutsche Forschungsgemeinschaft, Bad Honnef, Germany, June 18-20, 2006.

89. "Electronic structure of nitride surfaces", 28th International Conference on the Physics of Semiconductors, Vienna, Austria, July 24-28, 2006.
90. "Hydrogen in Semiconductors and Insulators", International Symposium on Metal-Hydrogen Systems, Lahaina, Maui, Hawaii, October 1-6, 2006.
91. "Electronic structure of nitride surfaces", 6th Akasaki Research Center Symposium, Nagoya University, October 19-20, 2006.
92. "Electronic structure of nitride surfaces", International Workshop on Nitride-Based Nanostructures, Berlin, Germany, February 5-7, 2007.
93. "Defect Engineering in Oxide Semiconductors", Spring Meeting of the Materials Research Society, Symposium F, San Francisco, California, April 9-13, 2007.
94. "Role of hydrogen at germanium/dielectric interfaces", 5th International Conference on Silicon Epitaxy and Heterostructures (ICSI-5), Marseille, France, May 20-25, 2007.
95. "Electronic structure of nitrides and pnictides", Pan American Advanced Study Institute on Electronic States and Excitations on Nanostructures, Zacatecas, Mexico, June 11-22, 2007.
96. "Controlling the conductivity of wide-band-gap semiconductors and oxides", Theory Meets Industry Workshop, Vienna, June 12-14, 2007.
97. "Effects of point defects and impurities on kinetics in hydrogen storage materials", Gordon Research Conference on Hydrogen-Metal Systems, Colby College, Waterville, Maine, July 9-13, 2007.
98. "Oxides as Semiconductors", Hong Kong-US Workshop on Advanced Materials, Hong Kong, September 12-14, 2007.
99. "Point Defects in ZnO and GaN", Workshop on Challenges facing ZnO and GaN, Virginia Commons Resort, Glenn Allen, Virginia, October 18-19, 2007.
100. "Hydrogen as an electronically active impurity: consequences for photoelectrolysis and hydrogen storage", Gordon Research Conference on Electrochemistry, Ventura, California, January 6-11, 2008.
101. "Role of defects in kinetics of hydrogen storage materials", Workshop on Inorganic Materials for Energy Conversion, Storage and Conservation, Lake Arrowhead, California, February 19-22, 2008.
102. "Effects of point defects and impurities on kinetics in hydrogen storage materials", APS March Meeting, New Orleans, Louisiana, March 10-14, 2008
103. "Electronic structure of nitride surfaces", Cambridge-UCSB Workshop on Organic and Inorganic Electronics, Cambridge, United Kingdom, April 13-16, 2008.

104. “Atomic and electronic structure of hydrogen-related centers in hydrogen storage materials”, 11th International Conference on Muon Spin Rotation, Relaxation and Resonance, Tsukuba, Japan, July 21-25, 2008.
105. “Defect control in oxides”, Gordon Research Conference on Defects in Semiconductors, Colby-Sawyer College, New London, NH, August 3-8, 2008.
106. “New insights in kinetics of hydrogen storage materials”, Materials Science and Technology Conference, Pittsburgh, PA, October 5-9, 2008.
107. “Oxides as Semiconductors”, CNSI-RIEC Workshop: Nanoelectronics, Spintronics and Photonics, Santa Barbara, CA, October 9-10, 2008.
108. “Defect Creation and Annihilation in GaN and ZnO”, Workshop on ‘Towards Reality in Nanoscale Materials’, Levi, Finland, December 3-5, 2008.
109. “How Hydrogen Keeps Surprising Us”, Symposium on Recent Advances in Materials Physics, Vanderbilt University, Nashville, TN, April 3-5, 2009.
110. “Oxides as Semiconductors”, Electronic Materials Symposium, Santa Clara, CA, April 10, 2009.
111. “First-principles studies of hydrogen-related defects in silicon”, First International Workshop on the Staebler-Wronski Effect, Berlin, Germany, April 20-22, 2009.
112. “Advances in Electronic Structure Methods for Defects and Impurities”, CECAM Workshop on Which electronic structure method for the study of defects?, Lausanne, Switzerland, June 8-10, 2009.
113. “Sources of Conductivity in Transparent Oxides”, Workshop on Computer Simulation of Oxides, Trinity College, Dublin, Ireland, September 9-11, 2009.
114. “Sources of doping for InN bulk and surfaces”, EMRS Fall Meeting, Warsaw, Poland, September 13-17, 2009.
115. “Impact of point defects and surfaces on the properties of nitride semiconductors”, 2nd UCSB-Tohoku Workshop: Nanoelectronics, Spintronics and Photonics, Sendai, Japan, October 22-23, 2009.
116. “Doping of InN and AlN bulk and surfaces”, Fall Meeting of the Materials Research Society, Boston, Massachusetts, November 30-December 4, 2009.
117. “Dangling bonds, hydrogen, and consequences for SiGe solar cells”, 2nd International Symposium on Innovative Solar Cells, Tsukuba, Japan, December 7-8, 2009.
118. “Role of point defects and additives in kinetics of hydrogen storage materials”, APS March Meeting, Portland, Oregon, March 15-19, 2010. [Unable to deliver due to injury.]

119. “Point Defects, Surfaces, and Loss Mechanisms in Nitrides”, Spring Meeting of the Materials Research Society, Symposium T, San Francisco, California, April 5-9, 2010.
120. “First-principles approaches for hydrogen storage materials”, Molecular Models for Carbon-Neutral Industrialization, Palm Desert, California, April 9-10, 2010.
121. “First-Principles Investigations of Point Defects”, Summer School on Computational Materials Science, San Sebastian, Spain, June 28- July 3, 2010.
122. **Plenary talk:** “Hydrogen in oxides and nitrides: Unexpected physics and impact on devices”, Europhysical Conference on Defects in Insulating Materials (EURODIM) Pécs, Hungary, July 12-16, 2010.
123. “Electronic structure of nitride alloys”, Psi_k 2010 Conference 2010, Berlin, Germany, September 12-16, 2010.
124. **Plenary talk:** “First-Principles Studies of Loss Mechanisms in Nitride LEDs and Lasers”, International Workshop on Nitrides, Tampa, FL, September 20-24, 2010.
125. “First-principles simulations of defects in oxides and nitrides”, School on Computational Modeling of Materials, Antwerp, Belgium, December 2-3, 2010.
126. “Missing dangling bonds and other mysteries: How germanium and hydrogen keep surprising us”, Haller Symposium, Berkeley, CA, June 18, 2011.
127. “Point Defects in Titania”, FIESTAE 2011, Frontiers in Interface Science: Theory and Experiment, Berlin, June 28 - July 1, 2011.
128. “Shallow or deep nature of acceptors in nitride semiconductors”, 9th International Conference on Nitride Semiconductors, Glasgow, UK, July 10-15, 2011.
129. “First-principles calculations for defects and impurities: hydrogen in oxides and nitrides”, Workshop on "Modern developments in the *ab initio* description of charged systems for semiconductors and electrochemistry", Ringberg Castle, Germany, October 24-26, 2011.
130. “First-Principles Studies of Loss Mechanisms in Nitride Light Emitters”, Conference on Computational Physics, Gatlinburg, TN, October 30-November 3, 2011.
131. “First-principles studies of the causes of droop”, SPIE Photonics West, San Francisco, CA, January 21-26, 2012.
132. “Loss Mechanisms in Nitride Light Emitters”, APS March Meeting, Boston, MA, February 27-March 2, 2012.
133. “Calculations of optical transitions within density functional theory”, Workshop on Quantum and Atomistic Modeling of Materials Defects, Institute for Pure and Applied Mathematics, University of California, Los Angeles, October 1-5, 2012.

134. “Fundamentals of n -type and p -type conducting oxides from first principles”, TCM-2012 (International Conference on Transparent Conducting Materials), Hersonissou, Crete, Greece, October 21-26, 2012.
135. “Hydrogen in Oxide Semiconductors”, Oxide TFT Workshop, Samsung Display, Gihung, Seoul, Korea, November 13, 2012.
136. “Conducting Oxides for Electronics and Optoelectronics”, Fall Meeting of the Materials Research Society, Boston, Massachusetts, November 26-30, 2012.
137. “First-principles studies of loss mechanisms in LEDs”, SPIE Photonics West, San Francisco, CA, February 2-7, 2013 (Presentation given by D. Steiauf).
138. “Complex oxides for next-generation electronics”, Spring Meeting of the Deutsche Physikalische Gesellschaft, Regensburg, Germany, March 11-15, 2013.
139. “Complex oxides for next-generation electronics”, 16th Brazilian Workshop on Semiconductor Physics, Itirapina, Brazil, May 6-10, 2013.
140. “Complex oxide interfaces”, 25th Annual Workshop on Recent Developments in Electronic Structure Theory, Williamsburg, Virginia, June 11-14, 2013.
141. “Defects at Ge and III-V interfaces”, 18th Conference on Insulating Films on Semiconductors (INFOS 2013), Cracow, Poland, June 25-28, 2013.
142. **Plenary talk:** “First-Principles Studies of Oxides for Electronics and Optoelectronics”, 7th Conference of the Asian Consortium on Computational Materials Science (ACCMS-7), Nakhon Ratchasima, Thailand, July 23-28, 2013.
143. **Plenary talk:** “Uncovering and surmounting loss mechanisms in nitride light emitters”, 10th International Conference on Nitride Semiconductors, Washington, DC, August 25-30, 2013.
144. “Complex oxides for charge-based electronics”, CECAM Workshop on *Functional Oxides for Emerging Technologies*, Bremen, Germany, October 14-18, 2013.
145. “Complex Oxide Interfaces: Conquering the (Polar) Catastrophe”, AVS 60th International Symposium, Long Beach, California, October 28-November 1, 2013.
146. “Controlling the conductivity of two-dimensional conductors”, Electronic Materials and Applications 2014, American Ceramic Society, Orlando, Florida, January 22-24, 2014.
147. “Doping and Defects in III-Nitrides”, UC Davis Engineering Research Center Workshop on “Electronics for Harsh Environments”, Davis, California, May 5, 2014.
148. “Point Defects in Nitride Semiconductors”, EMRS Spring Meeting, Lille, France, May 26-30, 2014.

149. “Fundamental limits on optical transparency of transparent conducting oxides”, 13th International Conference on Modern Materials and Technologies: 6th Forum on New Materials, Montecatini Terme, Italy, June 15-19, 2014 (Presentation given by Hartwin Peelaers).
150. “Effects of high doping in transparent conductors”, CECAM Workshop on *Nanostructured Zinc Oxide and related materials*, Bremen, Germany, June 23–27, 2014.
151. “Quantum computing with defects”, 8th International Conference on Physics and Applications of Spin Phenomena in Solids (PASPS VIII), Washington DC, July 28-31, 2014.
152. **Keynote talk:** “Complex oxides for charge-based electronics”, 9th International Conference on Computational Physics (ICCP9), National University of Singapore, Singapore, January 7-11, 2015.
153. “Transparent conductors for energy and electronics”, 9th International Conference on Computational Physics (ICCP9), National University of Singapore, Singapore, January 7-11, 2015.
154. “Absolute surface energies of nitride surfaces”, 2015 Lawrence Workshop on Epitaxy, Arizona State University, Tempe, Arizona, February 26-27, 2015.
155. “Impact of point defects on efficiency of nitride light emitters”, Spring Meeting of the Materials Research Society, Symposium FF, San Francisco, California, April 6-10, 2015.
156. “Defects as nonradiative recombination centers”, Workshop on “Nothing is perfect—The quantum mechanics of defects”, Ascona, Switzerland, April 26-29, 2015.
157. “Mott-Hubbard gap and optical properties of rare-earth titanates”, CNLS 35th Annual Conference on Electronic Structure Approaches & Applications to Quantum Matter, Santa Fe, New Mexico, May 18-21, 2015.
158. “Controlling the properties of two-dimensional conductors”, Workshop on Advances in Modeling of Nano Materials, Hefei, China, June 14-16, 2015.
159. “Optoelectronic materials: transparent conductors and light emitters”, Workshop on Density-Functional Theory and Beyond: First-Principles Simulations of Molecules and Materials, Berlin, Germany, July 13-23, 2015.
160. **Plenary talk:** “Impact of defects on efficiency of solid-state light emitters”, 28th International Conference on Defects in Semiconductors, Helsinki, Finland, July 26-31, 2015.
161. “Role of point defects, additives, and particle size in kinetics of hydrogen storage materials”, E-MRS Fall Meeting, Symposium A, Warsaw, Poland, September 15-18, 2015.
162. “Electronic structure and stability of charged complex oxide surfaces”, Workshop on Simulation of chemistry-driven growth phenomena for metastable materials, Rauschholzhausen, Germany, November 8-11, 2015.
163. “Impact of defects on efficiency of nitride devices”, Fall Meeting of the Materials Research Society, Boston, Massachusetts, November 30-December 4, 2015.

164. “Impact of defects on efficiency of nitride devices”, March Meeting of the American Physical Society, Baltimore, Maryland, March 14-18, 2016.
165. “Point defects, impurities, and small hole polarons in the rare-earth titanates”, Gordon Research Conference on Point Defects in Semiconductors, New London, New Hampshire, August 14-19, 2016.
166. “Radiative and nonradiative recombination at defects and impurities”, International Conference on Advanced Materials Modelling (ICAMM), Rennes, France, September 5-7, 2016.
167. “BN and its alloys as ultra-wide-band-gap materials for energy applications”, E-MRS Fall Meeting, Symposium L, Warsaw, Poland, September 19-22, 2016.
168. “First-principles modeling of ultra-wide-band-gap nitride semiconductors”, E-MRS Fall Meeting, Symposium F, Warsaw, Poland, September 19-22, 2016.
169. **Keynote talk:** “First-principles modeling of oxides: bulk properties and interfaces”, E-MRS Fall Meeting, Joint Session of Symposia C, M, and Z, Warsaw, Poland, September 19-22, 2016.
170. “Correct implementation of polarization constants in nitride semiconductors”, International Workshop on Nitride Semiconductors, Orlando, Florida, October 2-7, 2016.
171. “Role of excited states in recombination at defects and impurities”, NG Next Workshop on Physics of Light-matter Interactions & Excited State Dynamics, Redondo Beach, California, October 25-27, 2016.
172. “First-principles studies of single-photon emitters”, Fall Meeting of the Materials Research Society, Boston, Massachusetts, November 27-December 2, 2016.
173. **Keynote talk:** “First-principles studies of complex oxides and their interfaces”, 26th Annual Meeting of MRS-J, Yokohama, Japan, December 19-22, 2016.
174. **Keynote talk:** “First-principles studies of proton conductors”, 10th International Conference on Computational Physics (ICCP10), Macao, China, January 16 – 20, 2017.
175. “Electron-phonon interactions from first principles”, Invited Tutorial at March Meeting of the American Physical Society, New Orleans, Louisiana, March 12, 2017.
176. “Impact of electric fields on complex oxide heterostructures and surfaces”, Workshop on High electric Fields in Electrochemistry, Schloss Ringberg, Tegernsee, Germany, March 29-31, 2017.
177. “Using the right criteria for design and discovery”, APS *Physics Next* Workshop: Materials Design and Discovery, Riverhead, New York, May 15-17, 2017.
178. **Plenary talk:** “First-principles theory of wide-band-gap materials”, 59th Electronic Materials Conference, University of Notre Dame, June 28-30, 2017.

179. **Plenary talk:** “Wide-band-gap semiconductors: present and future”, 12th International Conference on Nitride Semiconductors, Strasbourg, France, July 24-28, 2017.
180. **Keynote talk:** “Turning SrTiO₃ into a Mott insulator”, IUMRS-ICAM: 15th International Conference on Advanced Materials, Kyoto, Japan, August 28-September 1, 2017.
181. “Impact of doping on proton conductivity in proton-conducting electrolytes”, E-MRS Fall Meeting, Symposium A, Warsaw, Poland, September 18-21, 2017.
182. “Impact of point defects on efficiency of nitride light emitters”, E-MRS Fall Meeting, Symposium P, Warsaw, Poland, September 18-21, 2017.
183. “Electronic and optical properties of rare-earth titanates”, International Workshop on Oxide Electronics, Chicago, Illinois, September 24-27, 2017.
184. “First-principles modeling of ultra-wide-band-gap nitrides”, International Workshop on UV Materials and Devices (IWUMD 2017), Fukuoka, Japan, November 14-18, 2017.
185. “Functional defects in battery electrodes”, Fall Meeting of the Materials Research Society, Boston, Massachusetts, November 26-December 1, 2017.
186. “First-principles modeling of gallium oxide and related semiconductors”, SPIE Photonics West, Conference 10533: *Oxide-based Materials and Devices IX*, San Francisco, California, January 27-February 1, 2018.
187. “Impact of point defects on efficiency of light emitters”, SPIE Photonics West, Conference 10554: *Light-Emitting Diodes: Materials, Devices, and Applications for Solid State Lighting XXII*, San Francisco, California, January 27-February 1, 2018.
188. “Role of excited states in recombination processes”, 3rd Annual Southern California Theoretical Chemistry Conference, Caltech, Pasadena, California, May 5, 2018.
189. “Electronic and optical properties of rare earth titanates”, 5th Workshop on Complex Oxides, Capri, Italy, May 20-24, 2018.
190. **Plenary Talk:** “Point defects and impurities in boron nitride”, 3rd International Conference on the Physics of 2D Crystals, La Valleta, Malta, May 29-June 2, 2018.
191. “Using the right criteria for design and discovery”, Lecture Series on Materials Theory and Computation In Honor of Prof. John P. Perdew for His 75th Birthday, Xi’an Jiaotong University, June 27-July 1, 2018.
192. “Ion-transport engineering of hydrogen-conducting electrolytes”, Thomas Young Centre 5th Energy Workshop “From Atoms to Applications”, London, UK, July 25-27, 2018.
193. “Wide-band-gap nitrides for quantum information applications”, 34th International Conference on the Physics of Semiconductors, Montpellier, France, July 29-August 3, 2018.

194. **Plenary Talk:** “Acceptors in nitrides: Doping, compensation, and impact on device performance”, 7th International Symposium on Growth of III-Nitrides, Warsaw, Poland, August 5-10, 2018.
195. “First-principles studies of transport and optical properties in sesquioxides”, CECAM Workshop on *Reliable and quantitative prediction of defect properties in Ga-based semiconductors*, Bremen, Germany, October 8-12, 2018.
196. “History of Defect Discovery”, OSA Incubator Meeting on *Defects by Design: Quantum Nanophotonics in Emerging Materials*, Washington, DC, October 28-30, 2018.
197. “Modeling Point Defects for Quantum Information Science”, 19th “Total Energy” workshop, International Center for Theoretical Physics, Trieste, January 9-11, 2019,
198. “Materials Design for long-wavelength LEDs”, 2019 U. S. Department of Energy Solid-State Lighting R&D Workshop, Dallas/Fort Worth, Texas, January 29–31, 2019.
199. “Defects and transport in oxide heterostructures”, March Meeting of the American Physical Society, Boston, MA, March 4-8, 2019.
200. “First-principles studies of loss mechanisms in light emitters”, 8th South African Conference on Photonic Materials (SACPM 2019), Kariega, East Cape, South Africa, May 6-10, 2019.
201. “First-Principles Modeling of Oxides”, GraFOx (Growth and Fundamentals of Oxides for Electronic Applications) Summer School, German-Italian Center for European Excellence, Villa Vigoni, Menaggio, Italy, June 3-9, 2019.
202. “Unusual Structures of Point Defects and Impurities in Sesquioxides”, 6th International Symposium on Advanced Microscopy and Theoretical Calculations (AMTC6), Nagoya, Japan, June 14-15, 2019.
203. “First-principles modeling of defects and hydrogen in oxides”, International Workshop on Models and Data for Plasma-Material Interaction in Fusion Devices (MoD-PMI 2019), National Institute for Fusion Science, Tajimi, Japan, June 18-20, 2019.
204. “Dopants and Defects in Ultrawide-Band-Gap Nitrides”, 13th International Conference on Nitride Semiconductors, Bellevue, Washington, July 7-12, 2019.
205. **Plenary talk:** “Quantum computing, transmitting, and sensing with defects”, 30th International Conference on Defects in Semiconductors, Seattle, Washington, July 21-26, 2019.
206. “First-principles studies of Ga₂O₃: defects, doping, and heterostructures”, 3rd International Workshop on Gallium Oxide and Related Materials (IWGO-3), The Ohio State University, Columbus, Ohio, August 12-15, 2019.

207. “Characterization of Point Defects in Semiconductors”, Tutorial at 4th International Workshop on Ultraviolet Materials and Devices (IWUMD4) St. Petersburg, Russia, September 8-9, 2019.
208. **Plenary Talk:** “Boron Nitride and Boron-Containing Nitride Alloys”, 4th International Workshop on Ultraviolet Materials and Devices (IWUMD4), St. Petersburg, Russia, September 8-9, 2019.
209. “First-principles studies of radiative and nonradiative recombination in halide perovskites”, e-conversion Conference 2019, Venice, Italy, September 9-13, 2019.
210. “First-principles studies of radiative and nonradiative recombination in halide perovskites”, E-MRS Fall Meeting, Symposium I, Warsaw, Poland, September 16-19, 2019.
211. “Fundamental limits on transparency of transparent conducting oxides”, Transparent Conductive Oxides—Fundamentals and Applications (TCO2019), Leipzig, Germany, September 23-27, 2019.
212. “Point Defects for Quantum Information Science”, AFOSR Workshop on Opportunities and Challenges for Quantum Materials, University of Chicago, October 8, 2019.
213. “Modeling Point Defects for Quantum Information Science”, Workshop on the Modeling of Defects, École Polytechnique, Palaiseau, France, October 18, 2019.
214. “Impact of small polarons on the properties of transition-metal oxides”, CECAM Workshop on “Polarons in the 21st Century”, Vienna, Austria, December 9-13, 2019.
215. “First-principles studies of defects, doping, and diffusion in gallium oxide”, SPIE Photonics West, Conference OE108: *Oxide-based Materials and Devices XI*, San Francisco, California, February 1-6, 2020.
216. “First-principles studies of radiative and nonradiative recombination in halide perovskites”, SPIE Photonics West, Conference OE126: *Light-Emitting Devices, Materials, and Applications XXIV*, San Francisco, California, February 1-6, 2020.
217. “Modeling Point Defects for Quantum Information Science”, Pittsburgh Quantum Institute Annual Meeting, Pittsburgh, Pennsylvania, April 15-17, 2020 (cancelled; talk moved to virtual seminar series: August 6, 2020).
218. **Keynote talk:** “Point defects in wide-band-gap semiconductors for quantum information applications”, Conference on Defects in Solids for Quantum Technologies (DSQT2020), Stockholm, Sweden, June 8-12, 2020 (cancelled; postponed to 2022).
219. “Role of Native Defects and Electronic Structure in the Performance of Transparent Conductors”, 15th International Ceramics Congress, Montecatini Terme, Italy, June 15-19, 2020 (cancelled; postponed to June 21-25, 2021).

220. “Impact of lattice relaxations on properties of point defects”, Workshop on First Principles Modeling of Defects in Solids: Charges meet Lattices”, Zurich, Switzerland, July 20-22, 2020 (cancelled; postponed to 2022)
221. “Point defects in wide-band-gap semiconductors for quantum information applications”, 35th International Conference on the Physics of Semiconductors, Sydney, Australia, August 9-14, 2020 (cancelled; postponed to June 26 – July 1, 2022).
222. “Boron nitride for quantum information applications”, International Workshop on Nitride Semiconductors, Berlin, Germany, August 23-28, 2020 (cancelled).
223. Invited tutorial: “Characterization and calculation of point defects”, International Workshop on Nitride Semiconductors, Berlin, Germany, August 23-28, 2020 (cancelled).
224. “Functional Defects in Materials”, Psi_k 2020 Conference, Lausanne, Switzerland, September 14-17, 2020 (cancelled; postponed to 2022).
225. “Simulation of radiative and non-radiative recombination in semiconductors”, Virtual Workshop on *Ab initio simulations supporting new materials & process developments*, 50th European Solid-State Device Research Conference & 46th European Solid-State Circuits Conference, September 14-15, 2020.
226. “Interfacing Scandium Nitride with GaN and AlN for Enhanced Performance”, Fall Meeting of the Materials Research Society, Symposium F.EL06: *Contacting Materials and Interfaces for Optoelectronic Devices*, 2020 Virtual MRS Spring/Fall Meeting, November 27-December 4, 2020.
227. “Exploring (and exploiting) the physics of ultra-wide-bandgap nitrides”, Humphreys Lecture, UK Nitrides Consortium Winter Meeting, January 7-8, 2021. (virtual)
228. “Doping of gallium oxide and aluminum gallium oxide alloys”, SPIE Photonics West Digital Forum, Conference OE108: *Oxide-based Materials and Devices XII*, March 6-11, 2021.
229. “Defect-assisted nonradiative recombination in halide perovskites”, March Meeting of the American Physical Society, March 15–19, 2021. (virtual)
230. “First-Principles Modeling of Efficiency of Halide Perovskites”, 21st International Meeting on Information Display (IMID 2021), Seoul, Korea, August 25-27, 2021. (virtual)
231. “Nonradiative recombination in halide perovskites”, E-MRS Fall Meeting, Symposium A, Warsaw, Poland, September 20-23, 2021. (virtual)
232. “Doping of gallium oxide and aluminum gallium oxide alloys”, E-MRS Fall Meeting, Symposium P, Warsaw, Poland, September 20-23, 2021. (virtual)
233. “Conductivity and transparency of gallium oxide (and related oxides)”, Symposium on Transparent Conductive Materials/Transparent Oxide and Related Materials for Electronics and Optics (TCM/TOEO) 2021 Virtual Meeting, October 18-19, 2021.

234. “Exploring (and exploiting) the physics of ultra-wide-bandgap nitrides”, ICMaSS-2021 (International Conference on Materials and Systems for Sustainability), Nagoya, Japan, November 4-6, 2021. (virtual)
235. “Exploiting Polarization for Energy-Efficient Devices”, Fall Meeting of the Materials Research Society, Symposium EN15, December 6-8, 2021. (virtual)
236. **Keynote talk:** “Controlled doping of gallium oxide and aluminum gallium oxide alloys”, Materials Research Meeting, Symposium D3, Yokohama, Japan, December 13-17, 2021. (virtual)
237. “First-principles studies of diffusion in gallium oxide”, SPIE Photonics West On Demand, Conference OE108: *Oxide-based Materials and Devices XIII*, February 21-27, 2022.