LIST OF PUBLICATIONS AND PRESENTATIONS

Chris G. Van de Walle

JOURNAL ARTICLES

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DISSERTATION

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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 AlGaN 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”, □k 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, Rauischholzhausen, 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 $SrTiO_3$ 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 Ga_2O_3: 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.

238. "Point defects in semiconductors for quantum technologies", MRS Spring Meeting, Symposium QT07, Honolulu, Hawaii, May 8-13, 2022.

239. "Defects in materials for energy storage and generation", Workshop on "Electronic structure of nanomaterials", Brookhaven National Laboratory, May 23, 2022. (virtual)

240. "First-principles calculations of shallow impurities", Workshop on "First-principles modeling of defects in solids: Charges meet lattices", ETH Zurich, Switzerland, June 13-15, 2022.

241. "Point defects in semiconductors for quantum technologies", Conference on Defects in Solids for Quantum Technologies (DSQT2020), Stockholm, Sweden, June 13-17, 2022.

242. "Role of Native Defects and Electronic Structure in the Performance of Transparent Conductors", 15th International Ceramics Congress (CIMTEC), Perugia, Italy, June 20-24, 2022.

243. **Plenary talk**: "First-principles modeling of efficiency of halide perovskites", 9th International Conference on Optical, Optoelectronic and Photonic Materials and Applications (ICOOPMA) & 14th Europhysical Conference on Defects in Insulating Materials (EuroDIM), Gent, Belgium, July 3-8 (2022).

244. "First-principles studies of radiative and nonradiative recombination mechanisms", Psi-k Conference 2022, SwissTech Convention Center, EPFL Lausanne, Switzerland, August 22-25, 2022.

245. "Point defects in semiconductors for quantum technologies", 2022 Computing in Engineering Forum, University of Wisconsin-Madison, September 20-21, 2022. (virtual)

246. "Characterization and calculation of point defects", Invited Tutorial, International Workshop on Nitride Semiconductors, Berlin, Germany, October 9-14, 2022.

247. **Keynote talk**: "Conductivity and transparency of gallium oxide", TCM-TOEO 2022 (8th International Symposium on Transparent Conductive Materials & 12th International Symposium on Transparent Oxide and Related Materials for Electronics and Optics), Hersonissos, Crete, Greece , October 16-21, 2022.

248. "First-Principles modeling of wurtzite ferroelectrics", US-Japan Seminar on Dielectric and Piezoelectric Materials, Charleston, South Carolina, November 13 - 16, 2022.

249. "Controlling defect-assisted nonradiative recombination in halide perovskites", Fall Meeting of the Materials Research Society, Symposium SF5, December 6-7, 2022. (virtual)

250. "Role of hydrogen in gallium oxide", SPIE Photonics West, Conference OE108: *Oxide-based Materials and Devices XIV*, San Francisco, California, January 28-February 2, 2023.

251. "Controlling doping in Ga_2O_3 and $AlGaO_3$ alloys", March Meeting of the American Physical Society, Las Vegas, Nevada, March 5-10, 2023.

252. "Role of the trap-assisted Auger-Meitner effect in nonradiative recombination", ACS Spring 2023 Meeting, Indianapolis, Indiana, March 26-30, 2023.

253. "First-principles studies of thermal conductivity in $AlGaO_3$ alloys", MRS Spring Meeting, Symposium SF03, San Francisco, California, April 10-14, 2023.

254. "Defect tolerance in halide perovskites—A first-principles perspective", MRS Spring Meeting, Symposium EL04, San Francisco, California, April 10-14, 2023.

255. "From Color Centers to Quantum Emitters: A Century of Point Defects", 32nd International Conference on Defects in Semiconductors, Rehoboth Beach, Delaware, September 10-15, 2023.

256. "Defect-Assisted Nonradiative Recombination in Nitrides", 14th International Conference on Nitride Semiconductors, Fukuoka, Japan, November 12-17, 2023.

257. "Surface reconstructions on bare and hydrogenated gallium oxide surfaces and consequences for growth", SPIE Photonics West, Conference OE108: *Oxide-based Materials and Devices XV*, San Francisco, California, January 27-February 1, 2024.

258. "First-principles modeling of AlScN and related materials", 35th Annual Workshop on Fundamental Physics of Ferroelectrics and Related Materials, Carnegie Institution for Science, Washington, DC, February 4-7, 2024.

259. **Keynote talk**: "Controlling doping in Ga_2O_3 and related alloys", 5th International Workshop on Gallium Oxide and Related Materials (IWGO 2024), Berlin, Germany, May 26-31, 2024.