

## Anderson Janotti

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### RESEARCH INTERESTS

- Computational methods in materials science
- Electronic structure and density functional theory
- High throughput techniques in materials simulations
- Renewable energy materials
- Transport and spectroscopic phenomena in solids
- Overcoming doping bottlenecks in wide-band-gap oxide and nitride semiconductors
- Impact of defects and impurities in solids
- Complex oxides and their heterostructures
- Metal/semiconductor nanostructures
- Resistive switching materials
- Two dimensional layered materials for electronics
- high-k dielectrics for novel MOS devices

### EMPLOYMENT RECORD

Assistant Professor Department of Materials Science & Engineering University of Delaware Newark, DE	July 2015 - present
Project Scientist Materials Department University of California Santa Barbara Santa Barbara, CA	July 2014 - June 2015
Associate Project Scientist Materials Department University of California Santa Barbara Santa Barbara, CA	March, 2010 - July 2014
Assistant Project Scientist Materials Department University of California Santa Barbara Santa Barbara, CA	September, 2004 - March, 2010
Research Associate Metals & Ceramics Division and Computational Materials Science Group Oak Ridge National Laboratory, Oak Ridge, TN	August, 2002 - September, 2004
Postdoctoral Researcher National Renewable Energy Laboratory, Golden, CO	January, 2000 - August, 2002

Lecturer  
Department of Mathematics and Engineering  
UniABC – Universidade do Grande ABC  
Santo Andre, SP, Brazil

February, 1996 -  
December, 1999

Research Assistant  
Department of Materials and Mechanics  
Institute of Physics, University of Sao Paulo  
Sao Paulo, SP, Brazil

August, 1995-  
January, 2000

## **EDUCATION**

Ph.D. in Physics  
Department of Materials and Mechanics, Institute of Physics,  
University of Sao Paulo, Sao Paulo, Brazil  
Advisor: Professor Adalberto Fazzio  
Thesis: “Electronic structure of defects in semiconductors”

January, 2000

BSc in Physics  
Institute of Physics  
University of Sao Paulo, Sao Paulo, SP, Brazil  
(Finished in record time of 3.5 years, while normal duration is 4 years)

July, 1994

## **AWARDS AND SCHOLARSHIPS**

2012 - UCSB - Solid State Lighting and Energy Center, Outstanding Researcher Achievement

2011 - ITN-RAINBOW - Outstanding Speaker at E-MRS Spring Meeting

1995-1999 - CNPq PhD student scholarship

## **TEACHING EXPERIENCE**

### **Teaching at the University of Delaware**

Fall 2015: 608 Structure and Properties of Materials I. 25 Students.

Spring 2016: 609 Structure and Properties of Materials II. 15 Students.

### **Teaching Contributions at UCSB**

**ECE-216B**, Professor responsible: Pierre Petroff -- Winter 2009. Taught two lectures on first-principles theory of doping and defects in semiconductors.

**ECE-216B**, Professor responsible: Pierre Petroff -- Fall 2008. Taught a lecture on theory of defects in semiconductors.

**MAT-288N**, Professor responsible: Chris. G. Van de Walle -- Fall 2007. Responsible for “hands-on research” part of the course on First-principles Calculations for Materials. Taught several lectures about the fundamentals and practical aspects of the computer code Abinit and guided students over the course of a 6-week period, helping in the execution of their research projects.

**MAT-228**, Professor responsible: Chris Van de Walle -- Fall 2006. Taught one lecture on Introduction to Computational Modeling of Materials

**MAT-200B**, Professor responsible: Chris Van de Walle -- Winter 2006. Prepared and taught one lecture on Electronic and Atomic Structure of Materials.

**MAT-288N**, Professor responsible: Chris Van de Walle -- Fall 2005. Prepared and taught three lectures on First-principles Calculations for Materials.

### Teaching 1996-1999

Lecturer at the University of ABC, Santo Andre, Brazil.

Taught Physics, Physics Lab, and Electrical Circuits for Mechanical Engineering students, and Statistics for Education and Biology students.

### Undergraduate Projects Directed at UCSB

Student	Project	Year
Michael Ford	Development of visualization tools in Computational Materials Science	Summer 2006
Cathal Leahy	Development of visualization tools in Computational Materials Science	Summer 2007
David Alexander Robinson	Electronic structure of complex oxides $ABO_3$	Summer 2011

### Graduate Projects Directed in the group of Prof. Chris G. Van de Walle (UCSB)

Student	Topics	Year
Justin Weber	Novel CMOS materials, Quantum computing with defects	2006-2010
Joel B. Varley	Oxides as semiconductors	2007-2011
Gareth B. Wilson-Short	Hydrogen storage materials	2008
Pakpoom Reunchan	Native point defects in $In_2O_3$ , Si-N pairs in GaAsN dilute alloys	2007-2009
Qimin Yang	Defects and doping on nitride devices	2009-2013

John L. Lyons	Doping in nitrides and oxides, High-k materials for CMOS applications	2008-2012
Cyrus Dreyer	Effects of strain and cracking in nitride nitride films, Spontaneous and piezoelectric polarization in nitrides	2009-2013
Luke Gordon	Defects in nitride-based devices, and qubits in wide-band gap semiconductors	2009-2014
Lars Bjaalie	Interfaces of complex oxides	2011-
Karthik Krishnaswamy	Complex oxide surfaces	2013-
Patrick McBride	Correlated complex oxide heterostructures	2013-
Jimmy Shen	Optical properties of complex oxides, First-principles calculations of Auger processes in semiconductors	2013-
Wennie Wang	Optical properties of $WO_3$	2013-
Michael Swift	Electron localization in $BaCeO_3$	2014-
<b>Student</b>	<b>Topics</b>	<b>Year</b>
Wennie Wang	Electrochromic materials	2014-
Michael Swift	Hydrogen-related Materials	2014-
Hiral Tailor	Dielectric materials for nitride power devices	2014-

### Graduate Degree Committee

<b>Student</b>	<b>Year Completed</b>	<b>Chair/ Member</b>	<b>Degree</b>
Pakpoom Reunchan	2009	Sukit Limpijumnong	PhD, Thesis defended at Suranaree University of Technology, Thailand
Lars Bjaalie,	2016	Chris G. Van de Walle	PhD, Thesis defended at the Materials Department, University of California Santa Barbara,

### Postdoctoral Scholars Supervised in the group of Prof. Chris G. Van de Walle (UCSB)

<b>Postdoc</b>	<b>Year</b>
Abhishek Singh	2006-2007
Amra Peles	2006
Khang Hoang	2008-2010
Naoto Umezawa	2007

Min Sik Park	2008
Flemming Ehlers	2008
Poul Moses	2009-2010
Lars Ismer	2009-2011
Daniel Steiauf	2009-
Hartwin Peelaers	2011-
Minseok Choi	2010-2013
Anindya Roy	2011-2013
John L. Lyons	2012-2014
Burak Himmetoglu	2012-
Jose Eduardo Padilha	2013
Cyrus Dreyer	2013-

## GRANTS AND CONTRACTS

Years	Source	Amount	Principal Investigator
2004	LDRD Oak Ridge National Laboratory, Novel Materials for Solid-State Lighting	\$125K	R. McKee and A. Janotti
2004-2005	LDRD Oak Ridge National Laboratory, Magnetization in Nanoparticles	\$480K	G. M. Stocks and A. Janotti
2011-2015	US Army Research Office First-principles Theory of Defects and Interfaces in Complex Oxides	\$400K	C.G. Van de Walle and A. Janotti
2015-2018	US Department of Energy - Basic Energy Sciences Synthesis and Observation of Emergent Phenomena in Heusler Compound Heterostructures	\$225K	C. Palmstrom and A. Janotti

## PROFESSIONAL ACTIVITIES

### Reviewing and Refereeing Activity

Since 2001, regularly refereed articles for several journals, including:

Nature Materials, Physical Review Letters, Physical Review B, Applied Physics Letters, Journal of Applied Physics, Europhysics Letters, Computational Materials Science, Journal of Chemical Physics, Physica Status Solidi (a) and (b), Journal of Physics: Condensed Matter, Materials Research Bulletin, Solid State Communications, New Journal of Physics, Philosophical Magazine, Chemical Physics Letters, Semiconductor Science and Technology, Organic Electronics, Nature Scientific Reports

## Reviewing proposals for Grant Agencies

National Science Foundation, Department of Energy - Basic Sciences, Petroleum Research Fund, Research Grants Council (RGC) of Hong Kong, Czech Science Foundation

## Special Appointments (*e.g.*, *Editorships*)

- Guest editor to Materials Research Society Symposium Proceedings, Vol. 1633, Oxide Semiconductors, (Cambridge University Press, 2014). [[doi](#)]
- Guest editor to “Functional Metal Oxide Nanostructures”, Springer Series in Materials Science, Volume 149 (Springer, New York, 2011). [[doi](#)]
- Guest editor to “Functional Metal-Oxide Nanostructures” Materials Research Society Symposium Proceedings, Vol. 1174, (Warrendale, PA, 2009).

## Organization of Symposia

03/2008	Dopants and Defects in Semiconductors, with E. E. Haller and M. Stavola	Focus Session at the 2008 American Physical Society March Meeting, New Orleans, LA
03/2009	Functional Metal Oxides Nanostructure, with J. Wu, Weiqiang Han, and H.-C. Kim	Symposium at the 2009 Materials Research Society Spring Meeting, San Francisco, CA
09/2010	Theory and simulation of nitrides, with D. Yoder	Topical session, International Workshop on Nitride Semiconductors (IWN2010), Tampa FL,
03/2012	Dopants and Defects in Semiconductors, with L. Brillson	Focus Session at the 2012 American Physical Society March Meeting, Boston, MA
12/2013	Oxide Semiconductors, with S. Durbin, T. Veal, and M. Grundman	Symposium at the 2013 Materials Research Society Fall Meeting, Boston, MA
12/2014	Oxide semiconductors, with T. Veal, O. Bierwagen, and M. Higashi	Symposium at the 2014 Materials Research Society Fall Meeting, Boston, MA

## SELECTED PUBLICATIONS (total of 166 publications, over 7000 citations, *h*-index=42)

1. A. Janotti and C. G. Van de Walle. Hydrogen multicentre bonds. *Nature Materials* **6**, 44 (2007). [[doi](#)] (>300 citations)
2. C. Freysoldt, B. Grabowski, T. Hickel, J. Neugebauer, G. Kresse, A. Janotti, and C. G. Van de Walle. First-principles calculations for point defects in solids. *Reviews of Modern Physics* **86**, 235 (2014). [[doi](#)]
3. A. Janotti and C. G. Van de Walle. Fundamentals of zinc oxide as a semiconductor. *Reports on Progress in Physics* **72**, 126501 (2009). [[doi](#)] (>550 citations)

4. A. Janotti and C. G. Van de Walle. Native point defects in ZnO. *Physical Review B* **76**, 165202 (2007). [[doi](#)] (>700 citations)
5. M. Setvin, C. Franchini, X. Hao, M. Schmid, A. Janotti, M. Kaltak, C. G. Van de Walle, G. Kresse, and U. Diebold. Direct View at Excess Electrons in TiO<sub>2</sub> Rutile and Anatase, *Physical Review Letters* **113**, 086402 (2014). [[doi](#)]
6. J. L. Lyons, A. Janotti, and C. G. Van de Walle. Shallow versus deep nature of Mg acceptors in nitride semiconductors. *Physical Review Letters* **108**, 156403 (2012). [[doi](#)] (>40 citations)
7. J. R. Weber, W. F. Koehl, J. B. Varley, A. Janotti, B. B. Buckley, C. G. Van de Walle, and D. D. Awschalom. Quantum computing with defects. *Proceedings of the National Academy of Sciences of the United States of America* **107**, 8513 (2010). [[doi](#)]

## INVITED ORAL PRESENTATIONS

1. “The role of vacancies and polarons in SrTiO<sub>3</sub>,” 28th International Conference on Defects in Semiconductors, 7/27-7/31, 2015, Espoo, Finland.
2. “Metal to insulator transition in ultrathin complex-oxide heterostructures”, *Electronic Materials and Applications*, 1/20-1/22, 2016, Orlando, FL, USA.
3. “Electronic and structural defects in SrTiO<sub>3</sub>”, American Physical Society March Meeting, San Antonio, TX, March 2015.
4. “Polarons in complex oxides”, ICMR Workshop on “Charged systems and solid/liquid interfaces from first principles”, University of California, Santa Barbara, CA, July 2014.
5. “Plane-wave methods for defects in solids”, Hands-on Summer School: Electronic Structure Theory for Materials and (Bio)molecules”, University of California, Los Angeles, CA, July 2014.
6. “Electronic structure of complex oxide interfaces”, 2014 Energy Material Technology, Cancun, Mexico, June 2014.
7. “Defects and Doping in oxide semiconductors”, The Eighth International Conference on the Science and Technology for Advanced Ceramics, Yokohama, Japan, June 2014.
8. “The role of defects in oxide semiconductors”, Collaborative Conference on Materials Research (CCMR) 2014, Incheon, Seoul, South Korea, June 2014.
9. “Defect Prediction and Measurement Techniques for Solar Energy Materials”, Tutorial at MRS Spring Meeting, San Francisco, CA, April 2014.
10. “Controlling the two-dimensional electron gas at complex oxide interfaces”, American Physical Society March Meeting, Denver, CO, March 2014.
11. “The role of native defects in the electrical conductivity of metal-oxide semiconductors”, AVS 60th International Symposium and Exhibition, Long Beach, CA, October 2013.
12. “First-principles studies of oxide semiconductors”, The 13th International Meeting on Information Display - IMID-13”, Daegu, Republic of Korea, August 2013.

13. "First-principles Studies of Complex Oxides and Their Heterostructures", Pohang University Science and technology, Pohang, Republic of Korea, August 2013.
14. "Controlling the 2DEG in complex-oxide heterostructures", Pulsan University, Busan, Republic of Korea, August 2013.
15. "Small poltroons in wide-band-gap oxide semiconductors", The 7th Conference of the Asian Consortium on Computational Materials Science (ACCMS-7), Nakhon Ratchasima, Thailand, July 2013.
16. "Controlling the two-dimensional electron gas at the interface of complex oxides", Materials Outreach Program, University of California, Santa Barbara, January, 2013.
17. "Bulk and interface properties from first-principles", II Workshop on the Physics of Complex Oxides, Mallorca, Spain, October, 2012.
18. "Challenges in controlling the conductivity in complex oxides", Gordon Research Conference (GRC) on Defects in Semiconductors, University of New England, Maine, August, 2012.
19. "Small polarons in semiconducting oxides", Inaugural International Conference of Young Researchers on Advanced Materials (IUMRS-ICYRAM 2012), Singapore, July, 2012.
20. "Structural and electronic defects in transition-metal oxide semiconductors", 7th International Symposium on Advanced Materials and Nanostructures (ISAMN), Sao Paulo, Brazil, May, 2012.
21. "Doping and defects in wide-band-gap oxide semiconductors", Materials Research Society, Fall Meeting, Boston, MA, November, 2011.
22. "First-principles calculations for TiO<sub>2</sub>", CompSurf 2011 - Computational Surface Science, Santa Barbara, CA, August, 2011.
23. "Controlling the conductivity in InN", E-MRS Spring Meeting, Nice, France, May, 2011.
24. "Native defects and hydrogen impurities in oxide semiconductors", 7th Petite Workshop on the Defect Chemical Nature of Advanced Materials for Energy, Norway, March, 2011.
25. "Causes of yellow luminescence in GaN", APS March Meeting, Dallas, TX, March, 2011.
26. "Studies of defects in semiconductors using density functional theory and beyond", XII Brazilian Summer School on Electronic Structure Methods, Brazilia, DF, Brazil, July 2010.
27. "Defects and doping in oxides: What we have learned so far", Workshop on "Bridging the gap between theory and experiment: which theoretical approaches are best suited to solve real problems in nanotechnology and biology?" Stanford University, CA, February, 2010.
28. "Effects of hydrogen impurities in oxide and nitride semiconductors", Colloquium, Suranaree Technological University, Thailand, August, 2009.
29. "Oxygen vacancies in oxides", 25<sup>th</sup> ICDS - International Conference on Defects in Semiconductors, S. Pettersburg, Russia, July, 2009.
30. "LDA+U and hybrid functionals applied to the study of defects in oxide and nitride semiconductors", Workshop on "Which Electronic Structure Method for the Study of Defects?" CECAM-HQ-EPFL, Lausanne, Switzerland, June, 2009.



31. "Doping and defects in oxide semiconductors", Invited talk, Latin American School On Computational Materials Science, Santiago, Chile, January, 2009.
32. "Hydrogen multicenter bond in oxide and nitride semiconductors", American Physical Society, March Meeting, Pittsburgh, PA, March, 2009.
33. "Hydrogen as a source of n-type conductivity in ZnO", 5th International Workshop on ZnO and Related Materials, Ann Arbor, MI, September, 2008.
34. "Band alignments at oxide semiconductor interfaces", 11<sup>th</sup> International Conference on the Formation of Semiconductor Interfaces, Manaus, Amazonas, Brazil, August, 2007.
35. "On the cause of unintentional n-type conductivity in ZnO", 14<sup>th</sup> Semiconducting and Insulating Materials Conference SIMC-XIV, University of Arkansas, Fayetteville, AR, May, 2007.
36. "Hydrogen Multicenter Bonds in Oxides", Colloquium, Physics Department, Brigham Young University, Provo, UT, February, 2007.
37. "Hydrogen Multicenter Bonds", Materials Outreach Program Symposium, University of California Santa Barbara, CA, January, 2007.
38. "Point Defects and Impurities in ZnO", Seminar, Oak Ridge National Laboratory, Oak Ridge, TN, January, 2007.
39. "Hydrogen multicenter bond in oxides", Colloquium, Materials Department, University of California, Santa Barbara, CA, October, 2006.
40. "LDA+*U* applied to oxide and nitride semiconductors", American Physical Society, March Meeting 2006, Baltimore MD, March, 2006.
41. "New insights into the role of native point defects in ZnO", 3<sup>rd</sup> International Conference on Materials for Advanced Technologies and 9<sup>th</sup> Conference on Advanced Materials, Suntec, Singapore, July, 2005.
42. "Defect physics in III-V dilute nitride alloys: the important role of hydrogen", Materials Research Society, Spring Meeting 2004, San Francisco, CA, April, 2004.
43. "Larger atoms diffuse faster: interdiffusion in Ni-base superalloys", Colloquium, California State University, Northridge, CA, March, 2004.
44. "Computational design of a new material for high-efficiency spin-polarized electron source", Seminar, Thomas Jefferson National Accelerator Facility, Newport News, VA, March, 2003.
45. "Design of 1-eV gap GaAsNBi dilute alloys for optoelectronics", Seminar, Oak Ridge National Laboratory, Oak Ridge, TN, May, 2002.
46. "Hydrogen effects on the electronic properties of dilute InGaAsN alloys", High Performance Photovoltaics Meeting, Denver CO, March, 2002.
47. "The pivotal role of nitrogen in stabilizing the H<sub>2</sub>\* complex in GaPN", Colloquium, Federal University of Uberlandia, MG, Brazil, February, 2001.
48. "Design of 1-eV band gap materials compatible with GaAs technology", Seminar, Institute of Physics, University of Sao Paulo, SP, Brazil, February, 2001.

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**List of Publications**

1. J. B. Varley, A. Janotti, and C. G. Van de Walle. “Defects in AlN as candidates for solid-state qubits”. *Physical Review B Rapid Communication* **93**, 161201(R) (2016). [[doi](#)]
2. L. Bjaalie, A. Janotti, K. Krishnaswamy, and C. G. Van de Walle. “Point defects, impurities, and small hole polarons in GdTiO<sub>3</sub>”. *Physical Review B* **93**, 115316 (2016). [[doi](#)]
3. K. Krishnaswamy, L. Bjaalie, B. Himmetoglu, A. Janotti, L. Gordon, and C. G. Van de Walle. “BaSnO<sub>3</sub> as a channel material in perovskite oxide heterostructures”. *Applied Physics Letters* **108**, 083501 (2016). [[doi](#)]
4. J. L. Lyons, K. Krishnaswamy, L. Gordon, A. Janotti, and C. G. Van de Walle. “Identification of Microscopic Hole-Trapping Mechanisms in Nitride Semiconductors”. *IEEE Electron Device Letters* **37**, 154 (2016) [[doi](#)]
5. N. Umezawa and A. Janotti. “Controlling the Electronic Structures of Perovskite Oxynitrides and their Solid Solutions for Photocatalysis”. *ChemSusChem* **9**, 1-6 (2016). [[doi](#)]
6. A. J. Hauser, E. Mikheev, A. Kajdos, and A. Janotti. “Small polaron-related recombination in Ba<sub>x</sub>Sr<sub>1-x</sub>TiO<sub>3</sub> thin films by cathodoluminescence spectroscopy”. *Applied Physics Letters* **108**, 2901 (2016). [[doi](#)]
7. B. Himmetoglu and A. Janotti, “Transport properties of KTaO<sub>3</sub> from first-principles,” *Journal of Physics.: Condensed Matter* **28**, 065502 (2016). [[doi](#)]
8. P. M. McBride, A. Janotti, C. E. Dreyer, B. Himmetoglu, and C. G. Van de Walle, “Effects of biaxial stress and layer thickness on octahedral tilts in LaNiO<sub>3</sub>,” *Applied Physics Letters* **107**, 261901 (2015). [[doi](#)]
9. E. Mikheev, A. J. Hauser, B. Himmetoglu, N. E. Moreno, A. Janotti, C. G. Van de Walle, S. Stemmer “Tuning bad metal and non-Fermi liquid behavior in a Mott material: Rare-earth nickelate thin films”, *Science Advances* **1**, 1500797 (2015). [[doi](#)]
10. M Swift, A. Janotti, and C. G. Van de Walle, “Small polarons and point defects in barium cerate,” *Physical Review B* **92**, 214114 (2015). [[doi](#)]
11. 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, “Observation by resonant angle-resolved photoemission of a critical thickness for 2-dimensional electron gas formation in SrTiO<sub>3</sub> embedded in GdTiO<sub>3</sub>,” *Applied Physics Letters* **107**, 231602 (2015). [[doi](#)]

12. H. Peelaers, K. Krishnaswamy, L. Gordon, D. Steiauf, A. Sarwe, A. Janotti, and C. G. Van de Walle, "Impact of electric-field dependent dielectric constants on two-dimensional electron gases in complex oxides", *Applied Physics Letters* **107**, 183505 (2015). [[doi](#)]
13. H. Peelaers, D. Steiauf, J. B. Varley, A. Janotti, and C. G. Van de Walle, "(In<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> alloys for transparent electronics," *Physical Review B* **92**, 085206 (2015). [[doi](#)]
14. K. Krishnaswamy, C. E. Dreyer, A. Janotti, and C. G. Van de Walle, "First-principles study of surface charging in LaAlO<sub>3</sub>/SrTiO<sub>3</sub> heterostructures," *Physical Review B* **92**, 085420 (2015). [[doi](#)]
15. L. Weston, A. Janotti, X. Y. Cui, B. Himmetoglu, C. Stampfl, and C. G. Van de Walle, "Structural and electronic properties of SrZrO<sub>3</sub> and Sr(Ti,Zr)O<sub>3</sub> alloys," *Physical Review B* **92**, 085201 (2015). [[doi](#)]
16. 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, "Determination of the Mott-Hubbard gap in GdTiO<sub>3</sub>," *Phys. Rev. B* **92**, 085111 (2015). [[doi](#)]
17. L. Gordon, A. Janotti, and C. G. Van de Walle, "Defects as qubits in 3C- and 4H-SiC," *Phys. Rev. B* **92**, 045208 (2015). [[doi](#)]
18. K. Krishnaswamy, C. E. Dreyer, A. Janotti, and C. G. Van de Walle. First-principles study of surface charging in LaAlO<sub>3</sub>/SrTiO<sub>3</sub> heterostructures. *Physical Review B* **92**, 085420 (2015). [[doi](#)]
19. L. Weston, A. Janotti, X. Y. Cui, B. Himmetoglu, C. Stampfl, and C. G. Van de Walle. Structural and electronic properties of SrZrO<sub>3</sub> and Sr(Ti,Zr)O<sub>3</sub> alloys. *Physical Review B* **92**, 085201 (2015). [[doi](#)]
20. L. Bjaalie, A. Verma, B. Himmetoglu, A. Janotti, S. Raghava, V. Protasenko, E. H. Steenbergen, D. Jena, S. Stemmer, and C. G. Van de Walle. Determination of the Mott-Hubbard gap in GdTiO<sub>3</sub>. *Physical Review B* **92**, 085111 (2015). [[doi](#)]
21. L. Gordon, J. B. Varley, J. L. Lyons, A. Janotti, and C. G. Van de Walle. Sulfur doping of AlN and AlGa<sub>N</sub> for improved n-type conductivity. *Physical Status Solidi - Rapid Research Letters* **9**, 462 (2015). [[doi](#)]
22. L. Gordon, A. Janotti, and C. G. Van de Walle. Defects as qubits in 3C- and 4H-SiC. *Physical Review B* **92**, 045208 (2015). [[doi](#)]

23. 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. Small hole polarons in rare-earth titanates. *Applied Physics Letters* **106**, 212103 (2015). [[doi](#)]
24. C. E. Dreyer, A. Janotti, and C. G. Van de Walle. Brittle fracture toughnesses of GaN and AlN from first-principles surface-energy calculations. *Applied Physics Letters* **106**, 212103 (2015). [[doi](#)]
25. J. L. Lyons, A. Alkauskas, A. Janotti, and C. G. Van de Walle. First-principles theory of acceptors in nitride semiconductors. *Physical Status Solidi B* **252**, 900 (2015). [[doi](#)]
26. H. D. Taylor, J. L. Lyons, M. Choi, A. Janotti, and C. G. Van de Walle. Carbon-induced trapping levels in oxide dielectrics. *Journal of Vacuum Science and Technology A* **33**, 01A120 (2015). [[doi](#)]
27. K. Khrishnaswamy, C. E. Dreyer, A. Janotti, and C. G. Van de Walle. Structure and energetics of LaAlO<sub>3</sub> (001) surfaces. *Physical Review B* **90**, 235436 (2014). [[doi](#)]
28. L. Gordon, A. Janotti, and C. G. Van de Walle, Hydrogen bonds in Al<sub>2</sub>O<sub>3</sub> as dissipative two-level systems in superconducting qubits, *Scientific Reports* **4**, 7590 (2014). [[doi](#)]
29. B. Himmetoglu, A. Janotti, H. Peelaers, A. Alkauskas, and C. G. Van de Walle. First-principles study of electron mobility in SrTiO<sub>3</sub>, *Physical Review B* **90**, 241204 (2014). [[doi](#)]
30. K. Hoang, A. Janotti, and C. G. Van de Walle. The role of native defects in the transport of charge and mass and the decomposition of Li<sub>4</sub>BN<sub>3</sub>H<sub>10</sub>, *Physical Chemistry Chemical Physics* **16**, 25314 (2014). [[doi](#)]
31. J. L. Lyons, D. Steiauf, A. Janotti, and C. G. Van de Walle. Carbon as a Shallow Donor in Transparent Conducting Oxides. *Physical Review Applied* **2**, 064005 (2014). [[doi](#)]
32. J. E. Padilha, H. Peelaers, A. Janotti, and C. G. Van de Walle. Nature and evolution of the band-edge states in MoS<sub>2</sub>: From monolayer to bulk. *Physical Review B* **90**, 205420 (2014). [[doi](#)]
33. L. Bjaalie, B. Himmetoglu, A. Janotti, and C. G. Van de Walle. Turning SrTiO<sub>3</sub> into a Mott insulator. *Physical Review B* **90**, 195117 (2014). [[doi](#)]
34. C. Freysoldt, B. Grabowski, T. Hickel, J. Neugebauer, G. Kresse, A. Janotti, and C. G. Van de Walle. First-principles calculations for point defects in solids. *Reviews of Modern Physics* **86**, 235 (2014). [[doi](#)]

35. M. Setvin, C. Franchini, X. Hao, M. Schmid, A. Janotti, M. Kaltak, C. G. Van de Walle, G. Kresse, and U. Diebold. Direct View at Excess Electrons in TiO<sub>2</sub> Rutile and Anatase, *Physical Review Letters* **113**, 086402 (2014). [[doi](#)]
36. B. Himmetoglu, A. Janotti, L. Bjaalie, and C. G. Van de Walle. Interband and polaronic excitations in YTiO<sub>3</sub> from first principles. *Physical Review B* **90**, 161102(R) (2014). [[doi](#)]
37. A. Janotti, J. B. Varley, M. Choi, and C. G. Van de Walle. Vacancies and small polarons in SrTiO<sub>3</sub>, *Physical Review B* **90**, 085202 (2014). [[doi](#)]
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