

Curriculum Vitae

Contact Information

Axel van de Walle
Assistant Professor
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Personal Information

Year of Birth: 1972
Citizenship: Canadian, US Permanent Resident.
Spoken and Written Languages: English and French

Education

Ph. D. in Materials Science and Engineering (MIT, 2000)
Title: The Effect of Lattice Vibrations on Substitutional Alloy Thermodynamics
Advisor: Prof. Gerbrand Ceder

Recent Professional Experience

Assistant Professor (July 2006–present)
Engineering and Applied Science Division,
California Institute of Technology.

Senior Research Associate (Jan 2004–June 2006)
Materials Science and Engineering, Chemistry and Physics Department,
Northwestern University
References: Mark Asta, Donald Ellis

Research Associate (Sep 2002–Dec 2003)
Post-doctoral Fellow (Sep 2000–Aug 2002)
Materials Science and Engineering Department, Northwestern University
Reference: Mark Asta

Grants

1. Principal Investigator for the project “CAREER: Extending the lattice stability framework in ab initio alloy thermodynamics” NSF Condensed Matter and Materials Theory program, DMR-0953378, (\$435,000/5 years).
2. Principal Investigator for the project “The Generalized Cluster Expansion: A Tool for Representing Structure-Property Relationships,” NSF Condensed Matter and Materials Theory program, DMR-0907669, (\$306,000/3 years).
3. Principal Investigator for the project “Computational design of high-melting-point materials”, ONR (\$250,000/1 yr, renewable for 3 yr).
4. Co-Principal Investigator, DOE’s Nuclear Energy Research Initiative (NERI) Project Number 08-051 (PI: Neils Gronbech Jensen, UC Davis). van de Walle’s share: \$449,000/3 years.
5. Principal Investigator, grant for Teragrid supercomputer time allocation (2003-2010, yearly). Allocation for 2010: 1 300 000 cpu-hour.
6. Senior Personnel in the “Center for the Predictive Modeling and Simulation of High Energy Density Dynamic Response of Materials” (PI: Michael Ortiz, Caltech). van de Walle’s share: \$1,000,000/5 years.
7. SEED funds from Caltech’s NSF Center for the Science and Engineering of Materials (CSEM): \$50,000/2 years.
8. Co-Principal Investigator on “Advanced Nanoscale Thin Film & Bulk Materials Towards Thermoelectric Power Conversion Efficiencies of 30%” (PI: Jeffrey Snyder). van de Walle’s share: ~\$25,000/1 year.

Prizes and Awards

1. Materials Research Society “Gold” Graduate Student Award (2000).
2. **Teaching Award** for the School of Engineering of MIT (1999). Each year, only one award is given for MIT’s entire School of Engineering.
3. “1967” Science and Engineering Doctoral Scholarship from the Natural Sciences and Engineering Research Council of Canada (1994–1998). Each year, about 50 “1967” scholarships are awarded throughout Canada.
4. Krashinsky award, awarded once per year by Quebec’s Association of Engineers (Ordre des Ingénieurs du Québec) (1993).
5. Industrial award R.A. Fessenden (1993).
6. Undergraduate level scholarship from the Natural Sciences and Engineering Research Council of Canada, for 3 consecutive years (1992-1994).
7. Canada Scholars, for 4 consecutive years (1990-1994).
8. Undergraduate program for integration to research (administered by École Polytechnique) (1993).

9. First price in Quebec at the pre-college level physics competition of the Canadian Association of Physicists (1990).

Professional activities

Associate Editor, *Calphad Journal*.

Developer of the Alloy Theoretic Automated Toolkit (ATAT), a software package available at <http://www.its.caltech.edu/~avdw/atat> that enables atomistic and thermodynamic modeling from first principles. ATAT is currently used by over 20 research groups in both industry and academia, including

- Greg Olson, Gautam Ghosh (Northwestern)
- Daryl Chrzan, Marvin Cohen, Steven Louie (Berkeley)
- Chris Woodward (Air Force Research Laboratory)
- Claudia Ambrosch-Draxl (University of Leoben)
- Chris Wolverton (Ford, now at Northwestern)
- Dane Morgan (University of Wisconsin)
- Long-Qing Chen and Zi-Kui Liu (Penn. State)
- Raymundo Arroyave (Texas A&M)
- Anton Van der Ven (U. Michigan)
- Vidvuds Ozoliņš (UCLA)
- Alex Zunger (NREL)
- Gerd Ceder (MIT)
- Ben Burton (NIST)
- Sundar Amancherla (GE)
- Mike Widom (Carnegie Mellon)
- Don Ellis (Northwestern)
- Gus Hart (Brigham Young)
- Dallas Trinkle (UIUC)
- Ralf Drautz (Oxford)
- William Schneider (Notre-Dame)

Co-organizer of *The Accelerated Implementation of Materials & Processes* Symposium at the 2004 *Materials Science & Technology* TMS-sponsored conference.

Referee for *Science*, *Nature*, *Nature Materials*, *Physical Review Letters*, *Acta Materialia*, *Calphad*, *Physical Review B*, *Physica B and C*, *Journal of Chemical Physics*, *Nanotechnology* and *Physica Status Solidi*.

Reviewer for DOE and NSF.

Presentations

Total number of contributed and invited talks: 40

Invited Talks

1. Ab initio above zero: Alloy thermodynamics from first principles, TMS annual meeting (forthcoming).
2. “Ab initio Description of Iron and Steel” seminar, Max-Planck-Institut für Eisenforschung (forthcoming).
3. The Alloy Theoretic Automated Toolkit, Berkeley (forthcoming).
4. Ab initio construction of structure-property relationships in crystals, APS March meeting (2010).
5. Building effective models from sparse but precise data, TMS annual meeting (2010).
6. Alloy thermodynamics without lattice stability?, TMS annual meeting (2010).
7. Ab Initio Thermodynamic Modeling of Multicomponent Alloys, MS&T and ACS combined meetings (2009).

8. Computational combinatorial screening and energy technologies, Harvard (2009).
9. The Alloy Theoretic Automated Toolkit, Texas A&M (2009).
10. Massively Parallel Architectures and Alloy Theory, TMS Annual meeting (2009).
11. Materials Science & Technology 2008, “Discovery and Optimization of Materials through Computational Design” Symposium, Pittsburgh (2008).
12. Recent additions to the Alloy Theoretic Automated Toolkit, Delft University of Technology, Netherlands (2008).
13. Automated crystal structure and surface reconstruction predictions from first-principles, Ciudad Universitaria, Madrid (2008).
14. Recent additions to the Alloy Theoretic Automated Toolkit, Air Force Research Lab (2008).
15. “Multiscale approach to alloys: advances and challenges” conference, Sweden (2007).
16. The tensorial cluster expansion, TMS Annual meeting (2007).
17. First-principles Calculations of Phonons Spectra in Disordered Alloys, TMS Annual meeting (2007).
18. Ab initio thermodynamics of Defective Oxide/Oxide Interfaces, University of Wisconsin (2006).
19. Ab initio above zero: Alloy thermodynamics from first principles, Ohio State University, Physics department (2006).
20. Ab initio thermodynamic modeling of multicomponent alloys, TMS 2006 Annual meeting.
21. First-Principles modeling of Ni-Ni₃Al interfaces at finite temperature, MRS 2005 Fall meeting.
22. Ab initio above zero: Alloy thermodynamics from first principles, Carnegie Mellon, Physics department (2005).
23. ATAT - A software toolkit for modeling coupled configurational and vibrational disorder in alloy systems, 2005 Summer School on Computational Materials Science, Materials Computation Center, University of Illinois at Urbana-Champaign.
24. Ab Initio Alloy Thermodynamics: Recent Progress and Future Directions, TMS 2004 Annual meeting.
25. Alloy Thermodynamics from First-Principles Calculations: Recent Progress and Future Directions, TMS 2003 Fall meeting (Materials Science & Technology 2003).
26. The Alloy Theoretic Automated Toolkit, seminar given at the National Institute of Standards and Technology (2003).
27. First-principles modelling of surface diffusion, Diffusion Workshop, National Institute of Standards and Technology (2003).
28. Automating Phase Diagram Calculations, TMS 2002 annual meeting.

29. The Importance of Lattice Vibrations in Substitutional Alloy Thermodynamics, American Physical Society Spring Meeting (1998).
30. Modeling Carbon Black Reinforcement in Rubber Compound, Semi-Annual Meeting of the American Chemical Society, Rubber Division, Pittsburg (1994).

Publications (preprints available at <http://www.its.caltech.edu/~avdw/pub.html>)

- [1] P. Tiwary, A. van de Walle, B. Jeon, and N. Gronbech-Jensen. Interatomic potentials for mixed oxide (MOX) nuclear fuels. 2010. submitted.
- [2] B. Meredig, A. Thompson, H.A. Hansen, C. Wolverton, and A. van de Walle. A method for locating low-energy solutions within DFT+U. 2010. submitted.
- [3] P. Dalach, D. E. Ellis, and A. van de Walle. First principles thermodynamic modeling of atomic ordering in yttria-stabilized zirconia. *Phys. Rev. B*, 2010. Accepted.
- [4] V.L. Vinograd, N. Paulsen, B. Winkler, and A. van de Walle. Thermodynamics of mixing in the ternary rhombohedral carbonate solid solution, $(\text{Ca}_x\text{Mg}_y\text{Mn}_{1-x-y})\text{CO}_3$, from atomistic simulations. *Calphad Journal*, 34:113, 2010.
- [5] E. Cockayne and A. van de Walle. Building effective models from scarce but accurate data: Application to an alloy cluster expansion model. *Phys. Rev. B*, 81:012104, 2010.
- [6] C. Ravi, A. van de Walle, B. K. Panigrahi, H. K. Sahu, and M. C. Valsakumar. Cluster expansion-monte carlo study of phase stability of vanadium nitrides. *Phys. Rev. B*, 81:104111, 2010.
- [7] A. van de Walle. **Invited paper:** First-principles alloy thermodynamics. In P. Derosa and T. Cagin, editors, *Multiscale Modeling: From Atoms to Devices*. CRC press, 2010. in production.
- [8] R. V. Chepulskii, W. H. Butler, A. van de Walle, and S. Curtarolo. Surface segregation in nanoparticles from first principles. *Scripta Materialia*, 62:179, 2010.
- [9] P. Tiwary, A. van de Walle, and N. Gronbech Jensen. Ab initio construction of interatomic potentials for uranium dioxide across all interatomic distances. *Phys. Rev. B*, 80:174302, 2009.
- [10] A. van de Walle. **Invited paper:** Multicomponent multisublattice alloys, nonconfigurational entropy and other additions to the Alloy Theoretic Automated Toolkit. *Calphad Journal*, 33:266, 2009.
- [11] R. Benedek, M. M. Thackeray, and A. van de Walle. Pourbaix-like phase diagram for lithium manganese spinels in acid. *J. Mat. Chem.*, 2009. Accepted.
- [12] O. Adjaoud, G. Steinle-Neumann, B.P. Burton, and A. van de Walle. First-principles phase diagram calculations for the HfC–TiC, ZrC–TiC, and HfC–ZrC solid solutions. *Phys. Rev. B*, 80:134112, 2009.
- [13] A. van de Walle. A complete representation of structure-property relationships in crystals. *Nature Materials*, 7:455, 2008 (Featured on the cover of the June 2008 issue).
- [14] R. Benedek and A. van de Walle. Reaction free energies of acid attack of lithium cobaltate. *Journal of the Electrochemical Society*, 155:A711, 2008.
- [15] R. Benedek, M. M. Thackeray, and A. van de Walle. Reaction free energy for proton-lithium ion exchange in lithium battery cathode materials. *Chem. Mater.*, 20:5485, 2008.

- [16] G. Ghosh, A. van de Walle, and M. Asta. First-principles calculations of properties of bcc, fcc and hcp solid solutions in Al-TM (TM = Ti, Zr, Hf) systems: A comparison between cluster expansion and supercell methods. *Acta Mater.*, 56:3202, 2008.
- [17] A. van de Walle and D. Ellis. First-principles thermodynamics of coherent interfaces in samarium-doped ceria nanoscale superlattices. *Phys. Rev. Lett.*, 98:266101, 2007.
- [18] D. Shin, A. van de Walle, Y. Wang, and Z.-K. Liu. First-principles study of ternary fcc solution phases from special quasirandom structures. *Phys. Rev. B*, 76:144204, 2007.
- [19] C. H. Lanier, A. van de Walle, N. Erdman, E. Landree, O. Warschkow, A. Kazimirov, K. R. Poeppelmeier, J. Zegenhagen, M. Asta, and L. D. Marks. The c(6x2) reconstruction on the SrTiO₃ (001) surface. *Phys. Rev. B*, 76:045421, 2007.
- [20] J. Z. Liu, G. Ghosh, A. van de Walle, and M. Asta. Transferable force-constant modeling of vibrational thermodynamic properties in fcc-based Al-TM (TM = Ti, Zr, Hf) alloys. *Phys. Rev. B*, 75:104117, 2007.
- [21] G. Ghosh, A. van de Walle, and M. Asta. First-principles phase stability calculations of pseudobinary alloys of (Al,Zn)₃Ti with L1₂, DO₂₂ and DO₂₃ structures. *Journal of Phase Equilibria and Diffusion*, 28:9, 2007.
- [22] B. Burton, A. van de Walle, and U. Kattner. First principles phase diagram calculations for the wurtzite-structure systems AlN-GaN, AlN-InN and GaN-InN. *J. Appl. Phys.*, 100:113528, 2006.
- [23] D. Shin, R. Arroyave, Z.-K. Liu, and A. van de Walle. Thermodynamic properties of binary hcp solution phases from special quasirandom structures. *Phys. Rev. B*, 74:024204, 2006.
- [24] R. Arroyave, A. van de Walle, and Z.-K. Liu. First-principles calculations of the Zn-Zr system. *Acta Materialia*, 54:473, 2006.
- [25] B.P. Burton and A. van de Walle. First principles phase diagram calculations for the system NaCl-KCl: the role of excess vibrational entropy. *Chemical Geology*, 225:222, 2006.
- [26] A. van de Walle. Genesis of crystal structures (in “news and views”). *Nature Materials*, 4:362, 2005.
- [27] A. van de Walle, G. Ghosh, and M. Asta. Ab initio modeling of alloy phase equilibria. In G. Bozzolo, R.D. Noebe, and P. Abel, editors, *Applied Computational Materials Modeling: Theory, Simulation and Experiment*. Kluwer Academic Publishers, 2005.
- [28] A. van de Walle and M. Asta. First-principles modeling of phase equilibria. In S. Yip, editor, *Handbook of Materials Modeling*, volume Part A. Springer, Dordrecht, the Netherlands, 2005.
- [29] J. Z. Liu, A. van de Walle, G. Ghosh, and M. Asta. Structure, energetics, and mechanical stability of Fe-Cu bcc alloys from first-principles calculations. *Phys. Rev. B*, 72:144109, 2005.
- [30] R. Benedek, A. van de Walle, S. Gerstl, M. Asta, D. N. Seidman, and C. Woodward. Partitioning of solutes in multiphase TiAl alloys. *Phys. Rev. B*, 71:094201, 2005.
- [31] A. van de Walle, Z. Moser, and W. Gasiot. First-principles calculation of the Cu-Li phase diagram. *Archives of Metallurgy and Materials*, 49:535, 2004.

- [32] M. J. Beck, A. van de Walle, and M. Asta. Surface energetics and structure of the Ge wetting layer on Si (100). *Phys. Rev. B*, 70:205337, 2004.
- [33] A. van de Walle, M. Asta, and P. W. Voorhees. First-principles calculation of the effect of strain on the diffusion of Ge adatoms on Si and Ge (001) surfaces. *Phys. Rev. B*, 67:041308(R), 2003.
- [34] E. Wu, G. Ceder, and A. van de Walle. Using bond-length-dependent transferable force constants to predict vibrational entropies in Au-Cu, Au-Pd, and Cu-Pd alloys. *Phys. Rev. B*, 67:134103, 2003.
- [35] B. Burton and A. van de Walle. First-principles-based calculations of the $\text{CaCO}_3\text{-MgCO}_3$ and $\text{CdCO}_3\text{-MgCO}_3$ subsolidus phase diagrams. *Physics and Chemistry of Minerals*, 30:88, 2003.
- [36] D. Morgan, B. Wang, G. Ceder, and A. van de Walle. First-principles study of magnetism in spinel MnO_2 . *Phys. Rev. B*, 67:134404, 2003.
- [37] D. Balachandran, D. Morgan, G. Ceder, and A. van de Walle. First-principles study of the structure of stoichiometric and Mn-deficient MnO_2 . *J. of Solid State Chemistry*, 173:462, 2003.
- [38] A. van de Walle and G. Ceder. The effect of lattice vibrations on substitutional alloy thermodynamics. *Rev. Mod. Phys.*, 74:11, 2002.
- [39] A. van de Walle, M. Asta, and G. Ceder. **Invited paper:** The Alloy Theoretic Automated Toolkit: A user guide. *CALPHAD Journal*, 26:539, 2002.
- [40] A. van de Walle and G. Ceder. Automating first-principles phase diagram calculations. *Journal of Phase Equilibria*, 23:348, 2002.
- [41] A. van de Walle and M. Asta. Self-driven lattice-model monte carlo simulations of alloy thermodynamic properties and phase diagrams. *Modelling Simul. Mater. Sci. Eng.*, 10:521, 2002.
- [42] A. van de Walle and M. Asta. First-principle investigation of perfect and diffuse anti-phase boundaries in hcp-based Ti-Al alloys. *Metallurgical and Materials Transactions A*, 33A:735, 2002.
- [43] G. Ghosh, A. van de Walle, M. Asta, and G.B. Olson. Phase stability of the Hf-Nb system: From first-principles to calphad. *CALPHAD Journal*, 26:491, 2002.
- [44] D. Morgan, D. Balachandran, G. Ceder, and A. van de Walle. A drastic influence of point defects on phase stability in MnO_2 . In M. Greenblatt, M.A. Alario-Franco, M.S. Whittingham, and G. Rohrer, editors, *MRS Proceedings*, volume 755, pages DD2.8–1, 2002.
- [45] H. Ramalingam, M. Asta, A. van de Walle, and J. J. Hoyt. Atomic-scale simulation study of equilibrium solute adsorption at alloy solid-liquid interfaces. *Interface Science*, 10:149, 2002.
- [46] A. van de Walle and G.Ceder. First-principles computation of the vibrational entropy of ordered and disordered Pd_3V . *Phys. Rev. B*, 61:5972, 2000.
- [47] D. Morgan, A. van de Walle, G. Ceder, J. D. Althoff, and D. de Fontaine. Vibrational thermodynamics: coupling of chemical order and size effects. *Modelling Simul. Mater Sci Eng.*, 8:295, 2000.

- [48] A. van de Walle and G. Ceder. Correcting overbinding in LDA calculations. *Phys. Rev. B*, 59:14992, 1999.
- [49] A. van de Walle, G. Ceder, and U. V. Waghmare. First-principles computation of the vibrational entropy of ordered and disordered Ni₃Al. *Phys. Rev. Lett.*, 80:4911, 1998.
- [50] A. van de Walle, C. Tricot, and M. Gerspacher. Modeling carbon black reinforcement in rubber compound. *Kautschuk Gummi Kunststoffe*, 49:172, 1996.