Contact Information

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Personal Information

Year of Birth: 1972
Citizenships: US, Canada, Belgium.
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

B. Eng. in Engineering Physics (École Polytechnique de Montréal, 1994)

Recent Professional Experience

Full Professor (July 2017–present)

Associate Professor (with tenure) (July 2011–June 2017)
School of Engineering,
Brown University.

Assistant Professor (July 2006–June 2011)
Department of Materials Science
Engineering and Applied Science Division,
California Institute of Technology.

Senior Research Associate (Jan 2004–June 2006)
(under the supervision of Mark Asta and Don Ellis)
Chemistry; Physics; Materials Science and Engineering Departments,
Northwestern University

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

Grants

Current

1. PI for project "High-throughput first-principles calculations of bulk and interfacial properties for the systematic exploration of the metastable material microstructure space", Army Research Office ($409,413/3 yr).
2. PI for project "CDS&E: Systematic exploration of the high entropy alloy space through high-dimensional thermodynamic modeling from high-throughput computations and experimental data", NSF ($379,741/3 yr).
3. PI for project "Designing practical metallic glasses through synergic computational and experimental exploration of the processing-structure-properties space", ONR ($3,200,000/4 yr, van de Walle's share: $800,000/4 yr) co-PI: Stefano Curtarolo (Duke), Douglas Hofmann (JPL), Jan Schroers (Yale).
4. co-PI for project "FMRG: Cyber: Material-on-demand manufacturing through convergence of manufacturing, AI and materials science", NSF, subcontract from Texas A&M University (van de Walle's share: $200,000/4 yr).
5. PI for project "Collaborative Research: Rare Earth Materials Under Extreme Conditions", NSF (van de Walle's share: $113,000/4 yr) Collaborators: Alex Navrotsky, Qijun Hong (ASU).
6. PI, grant for XSEDE supercomputer time allocation (2003-present, yearly) over 3,000,000 SU/yr awarded in latest cycle.

Previous

- Co-PI for project "Batch-wise Improvement in Reduced Design Space using a Holistic Optimization Technique (BIRDSHOT)", ARPA-e (van de Walle's share: $178,823/1.5 yr).
- PI for project "A high-throughput computational materials discovery and design framework for non-stoichiometric ceramics", Corning ($50,000/6 months).
- PI for project "SusChem: Collaborative Research: experimental and computational study of structure and thermodynamics of rare earth oxides above 2000 C", NSF (Collaborator: Alex Navrotsky, (PI for UC Davis team), van de Walle's share: $213,000, July 2018-June 2022).
- PI for project "Phase Equilibria in Li-Garnet Systems", Corning ($65,000/1 yr, Sept 2019-August 2020).
- PI for project "Accelerated Thermodynamic and Kinetic Modeling", ONR ($675,000/3 yr, February 2017-January 2020).
- co-PI for project "Designing Replacements for Strategic Structural Materials Through Rapid Computation and Experimentation", ONR, subcontract from UC Berkeley ($1,200,000 total, van de Walle's share: $390,000, October 2016-February 2019).
- PI for project "SusChem: Collaborative Research: experimental and computational study of structure and thermodynamics of rare earth oxides above 2000 C", NSF (Collaborator: Alex Navrotsky, (PI for UC Davis team), van de Walle's share: $285,000, July 2015-July 2018).
- PI for project "First-principle calculations of (111) APB energies in $L1_2$ Alloys in the presence of substitutional defects", US Air Force (via USAF at Leidos, Inc.) ($50,000, October 2015-October 2016).
- PI for project "Rapid Prototyping of Phase Diagrams", ONR ($675,000 total, October 2013-September 2017).
- PI for project "Combined Computational and Experimental Search for Isostructural Multicomponent Alloys - A Replacement Strategy for Refractory Materials", ONR ($1,050,000

total, van de Walle's share: $465,000, April 2012-March 2016, co-PI: Mark Asta and John Morris at UC Berkeley).
- PI 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 July 2010-July 2016).
- PI for project "First-principle Calculations of (111) APB Energies in Ni3Al in the Presence of Substitutional Defects", a contract with AFSOR at UES, Inc ($40,000 April 2013-April 2014).
- PI for project "New Theory and Algorithm development for Linear Scaling Electronic Structure Methods", ONR ($250,000 total, May 2014-December 2015).
- PI for project "Rational design of refractory materials; A combined computational and experimental approach", ONR ($750,000/3 yr, van de Walle's share $375,000 December 2010-April 2014, co-PI: Alexandra Navrotsky at UC Davis)
- PI for 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, beginning: September 15, 2009).
- PI for project "Computational Search for Isostructural Multicomponent Alloys — A Replacement Strategy for Refractory Materials", ONR ($250,000/1 yr, van de Walle's share: $150,000/1 yr, beginning: July 1, 2011, co-PI: Mark Asta).
- PI for project "Computational design of high-melting-point materials", ONR ($250,000/1 yr, beginning: April 1, 2010).
- Co-PI, 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.
- 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.
- SEED funds from Caltech's NSF Center for the Science and Engineering of Materials (CSEM): $50,000/2 years.
- Co-PI 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.

Current group members

- Xiao Han (PhD student)
- Prajna Jalagam (PhD student)
- Mina Bahadori (Undergraduate student)

Former group members (and job market outcome)

(Former members at Brown marked by "*")
Postdoctoral Fellows

* Siya Zhu (Post-doc at Texas A&M)
* Sayan Samanta (Senior Engineer at AspenTech)
* Chiraag Nataraj (Post-Doc at Sandia National Labs)
* Qijun Hong (Assistant Professor at Arizona State University)
* Ruoshi Sun (Computational Scientist at the University of Virginia)

* Sara Kadkhodaei (Assistant professor at the University of Illinois at Chicago)
* Pratyush Tiwary (Professor at the University of Maryland)
* Joseph Yasi (Senior Software Engineer at MathWorks)
* Ljubomir Miljacic (Entrepreneur)
- Ligen Wang (Professor, General Research Institute for Nonferrous Metals (China))
- Roman Chepulskyy (Staff Engineer, Samsung Semiconductor R&D)

Graduate Students

* Siya Zhu (see post-docs above)
* Hantong Chen (Post-doc at the University of Virginia)
* Helena Liu
* Sayan Samanta (see post-docs above)
* Chiraag Nataraj (see post-docs above)
* Sara Kadkhodaei (see post-docs above)
- Qijun Hong (see post-docs above)
- Pratyush Tiwary (see post-docs above)
- Gregory Pomrehn (Researcher at Boeing)
- Balaji Gopal Chirranjeevi (Scientist/Physicist at Illumina)
- Steven Demers (Data Scientist at Mitchell Madison Group)
- Adam Kowalski (Google)

Course Taught at Brown

- ENGN 0720 Thermodynamics
- ENGN 1410 Physical Chemistry of Solids
- ENGN 2410 Thermodynamics of Materials
- ENGN 2930 Atomistic Modeling of Materials

Professional activities

- Associate Editor, *Calphad Journal* (2009-present).
- Editorial Advisory Board, *Computational Materials Science* (2014-present)
- Developer of the Alloy Theoretic Automated Toolkit (ATAT), a software package available at `http://alum.mit.edu/www/avdw/atat` that enables atomistic and thermodynamic modeling from first principles. ATAT has now been interfaced with Biova's *Materials Studio*. ATAT has user base of over 1000 researchers in both industry and academia (see forum at `http://alum.mit.edu/www/avdw/forum`), including the following research groups:
  - Greg Olson, Gautam Ghosh (Northwestern)
  - Chris Wolverton (Ford, now Northwestern)
  - Chris Woodward (Air Force Research Laboratory)
  - Claudia Ambrosch-Draxl (University of Leoben)
  - Daryl Chrzan, Marvin Cohen, Steven Louie (Berkeley)
  - 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, now UCSB)
  - Vidvuds Ozoliņš (UCLA)
  - Alex Zunger (NREL, now U. Colorado)
  - Gerd Ceder (MIT, now UC Berkeley)
  - Ben Burton (NIST)
  - Sundar Amancherla (GE)
  - Mike Widom (Carnegie Mellon)
  - Don Ellis (Northwestern)
  - Gus Hart (Brigham Young)
  - Dallas Trinkle (UIUC)
  - Ralf Drautz (Oxford and U. Bochum)
  - William Schneider (Notre-Dame)

- Lead creator and maintainer of the Thermodynamic DataBase DataBase (TDBDB) a web search engine indexing all thermodynamic information available in a standardized "TDB" electronic format in the scientific literature: `https://alum.mit.edu/www/avdw/tdbdb.html`.
- Co-organizer of *The Accelerated Implementation of Materials & Processes* Symposium at the 2004 *Materials Science & Technology* TMS-sponsored conference.
- Co-organizer of the *International Research Conference on Structure and Thermodynamics of Oxides at High Temperature (STOHT16)*, October 21-22, 2016 Davis, CA.
- Referee (among others) for *Science*, *Nature*, *Nature Materials*, *Physical Review Letters*, *Acta Materialia*, *Calphad*, *Physical Review B*, *Physica B and C*, *Journal of Chemical Physics*, *Journal of Applied Physics*, *Nanotechnology*, *Computational Materials Science*, *Modelling and Simulation in Materials Science and Engineering* and *Physica Status Solidi*.
- Reviewer for DOE and NSF.
- Kaufman CALPHAD Scholarship Committee.

Service at Brown

- Undergraduate Concentration Advisor for the Materials group (2019-present).
- Graduate Representative for the Materials group (2013-2016, 2017-2019). This assignment includes handling graduate admissions (Masters and PhD) and recruitment activities, advising all Masters students and all PhD students not yet assigned to a thesis advisor.
- Materials faculty recruitment committee (2018).
- Undergraduate advising (freshman and sophomores, yearly).

Selected Invited Talks

1. Perfecting defect modeling: The science and engineering of refractory ceramics computational discovery and design, ACerS-MRS Virtual Workshop – Ceramic Materials in Extreme Environments: New Processing Tools and Data-Driven Approaches (Virtual) (2023).
2. Assessing phase diagram accuracy and high dimensional phase diagrams, UQPET Workshop III (Uncertainty Quantification for Phase Equilibria and Thermodynamics): Democratization of CALPHAD - Enabling Uncertainty Quantification (Virtual) (2023).
3. Computational Tools for the Generation and Visualization of High-Dimensional Phase Diagrams, Modern Materials Thermodynamics Symposium, MRS Annual Meeting (Virtual) (2022).
4. Critical inputs for CALPHAD, plenary talk at the 2021 Calphad Global conference (virtual) (2021).
5. Interfacing ab initio calculations, Calphad models, thermodynamic databases, web interfaces and visualization tools, BIOVIA Customer Conference (virtual) (2020).
6. Interfacing Ab Initio Calculations, CALPHAD Models and Data Science, Gordon Research Conference on Comparing Theories, Algorithms and Computation Protocols in Materials Science and Engineering, Newry, ME (2020, forthcoming).
7. Interfacing ab initio calculations, Calphad models, thermodynamic databases, web interfaces and visualization tools (Speaker: Sara Kadkhodaei), Hume-Rothery Symposium, TMS annual meeting, Phoenix, AZ (2019).
8. Software tools for high-throughput CALPHAD from first-principles data (speaker: Raymundo Arroyave), Keynote Lecture, Calphad Meeting, St-Malo, France (2018).

9. Software tools for high-throughput CALPHAD from first-principles data (speaker: Qijun Hong), Hume-Rothery Symposium, TMS annual meeting, Phoenix, AZ (2017).
10. Rapid Prototyping of Phase diagrams, TMS annual meeting (2015).
11. Accelerated molecular dynamics simulation via SISYPHUS, TMS annual meeting (2014).
12. Extending the lattice stability framework in ab initio alloy thermodynamics, Hume-Rothery Symposium, TMS Annual Meeting, San Antonio (2013).
13. Efficient modeling of solid phases: From thermodynamics to kinetics, Harvard University (2012).
14. Cluster expansion methods - progress and outlook, TMS annual meeting (2012).
15. Ab initio thermodynamics and energy materials design, Columbia University (2011).
16. Ab initio above zero: Alloy thermodynamics from first principles, TMS annual meeting (2011).
17. "Ab initio Description of Iron and Steel" symposium, Max-Planck-Institut für Eisenforschung (2010).
18. Ab initio construction of structure-property relationships in crystals, APS March meeting (2010).
19. Building effective models from sparse but precise data, TMS annual meeting (2010).
20. Alloy thermodynamics without lattice stability?, TMS annual meeting (2010).
21. Ab Initio Thermodynamic Modeling of Multicomponent Alloys, MS&T and ACS combined meetings (2009).
22. Computational combinatorial screening and energy technologies, Harvard (2009).
23. The Alloy Theoretic Automated Toolkit, Texas A&M (2009).
24. Massively Parallel Architectures and Alloy Theory, TMS Annual meeting (2009).
25. Materials Science & Technology 2008, "Discovery and Optimization of Materials through Computational Design" Symposium, Pittsburgh (2008).
26. Recent additions to the Alloy Theoretic Automated Toolkit, Delft University of Technology, Netherlands (2008).
27. Automated crystal structure and surface reconstruction predictions from first-principles, Ciudad Universitaria, Madrid (2008).
28. Recent additions to the Alloy Theoretic Automated Toolkit, Air Force Research Lab (2008).
29. "Multiscale approach to alloys: advances and challenges" conference, Sweden (2007).
30. The tensorial cluster expansion, TMS Annual meeting (2007).
31. First-principles Calculations of Phonons Spectra in Disordered Alloys, TMS Annual meeting (2007).
32. Ab initio thermodynamics of Defective Oxide/Oxide Interfaces, University of Wisconsin (2006).
33. Ab initio above zero: Alloy thermodynamics from first principles, Ohio State University, Physics department (2006).
34. Ab initio thermodynamic modeling of multicomponent alloys, TMS 2006 Annual meeting.
35. First-Principles modeling of Ni-Ni_3Al interfaces at finite temperature, MRS 2005 Fall meeting.
36. Ab initio above zero: Alloy thermodynamics from first principles, Carnegie Mellon, Physics department (2005).
37. 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-Champain.
38. Ab Initio Alloy Thermodynamics: Recent Progress and Future Directions, TMS 2004 Annual meeting.
39. Alloy Thermodynamics from First-Principles Calculations: Recent Progress and Future Directions, TMS 2003 Fall meeting (Materials Science & Technology 2003).

40. The Alloy Theoretic Automated Toolkit, seminar given at the National Institute of Standards and Technology (2003).
41. First-principles modelling of surface diffusion, Diffusion Workshop, National Institute of Standards and Technology (2003).
42. Automating Phase Diagram Calculations, TMS 2002 annual meeting.
43. The Importance of Lattice Vibrations in Substitutional Alloy Thermodynamics, American Physical Society Spring Meeting (1998).
44. Modeling Carbon Black Reinforcement in Rubber Compound, Semi-Annual Meeting of the American Chemical Society, Rubber Division, Pittsburg (1994).

Prizes, Awards and press coverage

1. "Highly cited Research certficate" from Elsevier, for the paper "Efficient stochastic generation of special quasirandom structures", which is the most cited paper published since 2013 in the CALPHAD journal (2016). Same paper is also a "Highly cited paper" according to the ISI (top 1% in field) (2018).
2. Paper "Prediction of the material with highest known melting point from ab initio molecular dynamics calculations" featured in the Washington Post, the Daily Mail, IEEE Spectrum, among other popular journals (2015).
3. "Top Cited Author" Elsevier certificate for the article "Multicomponent multisublattice alloys, nonconfigurational entropy and other additions to the Alloy Theoretic Automated Toolkit" in the Calphad Journal (2011).
4. NSF CAREER grant (2010).
5. Materials Research Society "Gold" Graduate Student Award (2000).
6. Teaching Award for the School of Engineering of MIT (1999). Each year, only one award is given for MIT's entire School of Engineering.
7. "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.
8. Krashinsky award, awarded once per year by Quebec's Association of Engineers (Ordre des Ingénieurs du Québec) (1993).
9. Industrial award R.A. Fessenden (1993).
10. Undergraduate level scholarship from the Natural Sciences and Engineering Research Council of Canada, for 3 consecutive years (1992-1994).
11. Canada Scholars, for 4 consecutive years (1990-1994).
12. First price in Quebec at the pre-college level physics competition of the Canadian Association of Physicists (1990).

Publications

Preprints available at http://alum.mit.edu/www/avdw/pub.html
ResearchID profile: http://www.researcherid.com/rid/L-5676-2013
Google Scholar page https://scholar.google.com/citations?user=urxZqnIAAAAJ

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[2] S. Samanta and A. van de Walle. Software tools for integrating special quasirandom structures and the cluster variation method into the calphad formalism. *J. of Phase Equilibria and Diffusion*, Sep, 2024. doi: 10.1007/s11669-024-01151-6.

[3] S. V. Ushakov, Q.-J. Hong, A. Pavlik III, A. van de Walle, and A. Navrotsky. Thermal expansion and enthalpies of phase transformation and fusion of Er_2O_3 and Tm_2O_3 from experiment and computation. *Chem. Mater.*, 36:4868, 2024. doi: 10.1021/acs.chemmater.4c00783.

[4] Q.-J. Hong, P. D. Tepesch, and A. van de Walle. Combined experimental and computational assessment of the Li_2O-La_2O_3-ZrO_2 phase diagram. *Journal of the American Ceramic Society*, 107:5682, 2024. doi: 10.1111/jace.19846.

[5] C. Kunselman, B. J. Bocklund, A. van de Walle, R. Otis, and R. Arroyave. Analytically differentiable metrics for phase stability. *Calphad Journal*, 86:102705, 2024. doi: 10.1016/j.calphad.2024.102705.

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[8] B. L. Brugman, Y. Han, L. J. Leinbach, K. Leinenweber, A. van de Walle, S. V. Ushakov, Q.-J. Hong, and A. Navrotsky. Computationally led high pressure synthesis and experimental thermodynamics of rock salt yttrium monoxide. *Chemistry of Materials*, in press, 2024. doi: 10.1021/acs.chemmater.3c02166.

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[12] Q. Hong, A. van de Walle, S. V. Ushakov, and A. Navrotsky. Integrating computational and experimental thermodynamics of refractory materials at high temperature. *Calphad journal*, 79:102500, 2022. doi: 10.1016/j.calphad.2022.102500.

[13] H. Liu and A. van de Walle. Rapid geometric screening of low-energy surfaces in crystals. *Symmetry*, 14:2067, 2022. doi: 10.3390/sym14102067.

[14] C. Oses, M. Esters, D. Hicks, S. Divilov, H. Eckert, R. Friedrich, M. J. Mehl, A. Smolyanyuk, X. Campilongo, A. van de Walle, J. Schroers, A. G. Kusne, I. Takeuchi, E. Zurek, M. Buongiorno Nardelli, M. Fornari, Y. Lederer, O. Levy, C. Toher, and S. Curtarolo. aflow++: a c++ framework for autonomous materials design. *Comput. Mat. Sci.*, 217:111889, 2022. doi: 10.1016/j.commatsci.2022.111889.

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[16] A. van de Walle, H. Chen, H. Liu, C. Nataraj, S. Samanta, S. Zhu, and R. Arroyave. Interactive exploration of high-dimensional phase diagrams. *JOM - J. Min. Met. Mat. S.*, 74:3478, 2022. doi: 10.1007/s11837-022-05314-z.

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[18] E. Y. Cramer et al. Evaluation of individual and ensemble probabilistic forecasts of covid-19 mortality in the US. *Proceedings of the National Academy of Science*, 119:e211356111, 2022. doi: 10.1073/pnas.2113561119.

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[22] H. Chen, Q.-J. Hong, S. Ushakov, A. Navrotzky, and A. van de Walle. A simple method for computing the formation energies of metal oxides. *Comput. Mat. Sci.*, 198:110692, 2021. doi: 10.1016/j.commatsci.2021.110692.

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[24] S. Samanta and A. van de Walle. Rapid screening of high-throughput ground state predictions. *Calphad*, 74:102306, 2021. doi: 10.1016/j.calphad.2021.102306.

[25] C. Nataraj, A. van de Walle, and A. Samanta. Temperature-dependent configurational entropy calculations for refractory high-entropy alloys. *Journal of Phase Equilibria and Diffusion*, 2021. doi: 10.1007/s11669-021-00879-9.

[26] Q. Hong, J. Schroer, D. Hofmann, S. Curtarolo, M. Asta, and A. van de Walle. Theoretical prediction of melting temperature for a Mo-Ru-Ta-W HCP multi-principal element alloy. *NPJ Computational Materials*, 7:1, 2021. doi: 10.1038/s41524-020-00473-6.

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[32] A. van de Walle and M. Asta. High-throughput calculations in the context of alloy design. *MRS Bull.*, 44:252, 2019. doi: 10.1557/mrs.2019.71.

[33] A. van de Walle and Q.-J. Hong. Assessing phase diagram accuracy. *J. Phase Equilib. Diff.*, 40:170, 2019. doi: 10.1007/s11669-019-00711-5.

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[35] S. Kadkhodaei and A. van de Walle. Software tools for thermodynamic calculation of mechanically unstable phases from first-principles data. *Comput. Phys. Commun.*, 246:106712, 2019. doi: 10.1016/j.cpc.2019.01.008.

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