

# Papers sorted by topic

Axel van de Walle

March 7, 2021

## Alloy Theoretic Automated Toolkit

- [1] P. Dalach, D. E. Ellis, and A. van de Walle. Adaptive cluster expansions and redox-dependent atomic ordering. *Comp. Mater. Sci.*, 83:207, 2014. Download: [\[DOI\]](#) [\[Cite\]](#) .
- [2] A. van de Walle. Methods for first-principles alloy thermodynamics. *JOM - J. Min. Met. Mat. S.*, 65:1523–1532, 2013. Download: [\[DOI\]](#) [\[Cite\]](#) .
- [3] A. van de Walle, P. Tiwary, M. M. de Jong, D. L. Olmsted, M. D. Asta, A. Dick, D. Shin, Y. Wang, L.-Q. Chen, and Z.-K. Liu. Efficient stochastic generation of special quasirandom structures. *Calphad*, 42:13–18, 2013. Download: [\[DOI\]](#) [\[Cite\]](#) .
- [4] 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. Download: [\[DOI\]](#) [\[Cite\]](#) [\[arXiv\]](#).
- [5] A. van de Walle. Multicomponent multisublattice alloys, nonconfigurational entropy and other additions to the Alloy Theoretic Automated Toolkit. *Calphad*, 33:266–278, 2009. Download: [\[DOI\]](#) [\[Cite\]](#) [\[arXiv\]](#).
- [6] A. van de Walle. A complete representation of structure-property relationships in crystals. *Nat. Mater.*, 7:455–458, 2008. Download: [\[DOI\]](#) [\[Cite\]](#) [\[Featured on cover\]](#) [\[See associated “News and Views” piece by Gus Hart\]](#).
- [7] A. van de Walle, M. D. Asta, and G. Ceder. The Alloy Theoretic Automated Toolkit: A user guide. *Calphad*, 26:539–553, 2002. Download: [\[DOI\]](#) [\[Cite\]](#) [\[arXiv\]](#).
- [8] A. van de Walle and G. Ceder. Automating first-principles phase diagram calculations. *J. Phase Equilib.*, 23:348–359, 2002. Download: [\[DOI\]](#) [\[Cite\]](#) [\[arXiv\]](#) [\[PDF 1173 KB\]](#) [\[PDF 2701 KB\]](#) [\[paper errata \(preprint ok\)\]](#).
- [9] A. van de Walle and M. D. Asta. Self-driven lattice-model monte carlo simulations of alloy thermodynamic properties and phase diagrams. *Model. Simul. Mater. Sc.*, 10:521, 2002. Download: [\[DOI\]](#) [\[Cite\]](#) [\[arXiv\]](#).

## CALPHAD method

- [10] S. Zhu and A. van de Walle. Computational assessment of novel predicted compounds in the Ni-Re alloy system. *J. of Phase Equilibria*, submitted, 2020.
- [11] S. Samanta and A. van de Walle. Rapid screening of high-throughput ground state predictions. *Calphad*, submitted, 2020.
- [12] A. van de Walle, J. Sabisch, A. M. Minor, and M. D. Asta. Identifying rhenium substitute candidate multi-principal-element alloys from electronic structure and thermodynamic criteria. *Journal of Materials Research*, 34:3296, 2019. Download: [\[DOI\]](#) [\[Cite\]](#) [\[Full text\]](#).
- [13] A. van de Walle and M. Asta. High-throughput calculations in the context of alloy design. *MRS Bull.*, 44:252, 2019. Download: [\[DOI\]](#) [\[Cite\]](#) .

- [14] A. van de Walle and Q.-J. Hong. Assessing phase diagram accuracy. *J. Phase Equilib. Diff.*, 40:170, 2019. Download: [DOI] [Cite] .
- [15] A. van de Walle, C. Nataraj, and Z.-K Liu. The thermodynamic database database. *Calphad*, 61:173, 2018. Download: [DOI] [Cite] .
- [16] A. van de Walle, R. Sun, Q.-J. Hong, and S. Kadhodaei. Software tools for high-throughput calphad from first-principles data. *Calphad*, 58:70, 2017. Download: [DOI] [Cite] .
- [17] G. Ghosh, A. van de Walle, M. D. Asta, and G.B. Olson. Phase stability of the Hf-Nb system: From first-principles to CALPHAD. *Calphad*, 26:491, 2002. Download: [DOI] [Cite] .

## Liquids

- [18] 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. Download: [DOI] [Cite] .
- [19] Q.-J. Hong and A. van de Walle. Re-entrant melting of sodium, magnesium and aluminum: General trend. *Phys. Rev. B Rapid Communications*, 100:140102(R), 2019. Download: [DOI] [Cite] [arXiv].
- [20] Q.-J. Hong and A. van de Walle. A user guide for SLUSCHI (solid and liquid in ultra small coexistence with hovering interfaces). *Calphad*, 52:88, 2016. Download: [DOI] [Cite] .
- [21] Q.-J. Hong and A. van de Walle. Solid-liquid coexistence in small systems: A statistical method to calculate melting temperatures. *J. Chem. Phys.*, 139:094114, 2013. Download: [DOI] [Cite] .
- [22] Q.-J. Hong and A. van de Walle. Direct first-principles chemical potential calculations of liquids. *J. Chem. Phys.*, 137:094114, 2012. Download: [DOI] [Cite] .
- [23] L. G. Wang and A. van de Walle. Ab initio calculations of the melting temperatures of refractory bcc metals. *Phys. Chem. Chem. Phys.*, 14:1529, 2012. Download: [DOI] [Cite] .
- [24] L. G. Wang, A. van de Walle, and D. Alfè. Melting temperature of tungsten from two ab initio approaches. *Phys. Rev. B*, 84:092102, 2011. Download: [DOI] [Cite] .

## Accelerated Molecular Dynamics

- [25] S. Kadhodaei and A. van de Walle. A simple local expression for the prefactor in transition state theory. *J. Chem. Phys.*, 150:144105, 2019. Download: [arXiv] [DOI] [Cite] .
- [26] P. Tiwary and A. van de Walle. A review of enhanced sampling approaches for accelerated molecular dynamics. In G. Tucker and C. Weinberger, editors, *Multiscale materials modeling for nanomechanics*. Springer, 2016. Download: [DOI] [Cite] .
- [27] A. van de Walle. Simulations provide a rare look at real melting (in “perspectives”). *Science*, 346:704, 2014. Download: [DOI] [Cite] [Full text].
- [28] P. Tiwary and A. van de Walle. Accelerated molecular dynamics simulations through stochastic iterations and collective variable based basin identification. *Phys. Rev. B*, 87:094304, 2013. Download: [DOI] [Cite] [arXiv].
- [29] P. Tiwary and A. van de Walle. Hybrid deterministic and stochastic approach for efficient long time scale atomistic simulations. *Phys. Rev. B*, 84:100301(R), 2011. Download: [DOI] [Cite] [arXiv].

## Mechanical Instabilities

- [30] S. Kadkhodaei and A. van de Walle. Software tools for thermodynamic calculation of mechanically unstable phases from first-principles data. *Comput. Phys. Commun.*, page 106712, 2019. Download: [DOI] [Cite] .
- [31] A. van de Walle. Reconciling SGTE and ab initio enthalpies of the elements. *Calphad*, 60:1, 2018. Download: [DOI] [Cite] .
- [32] S. Kadkhodaei and A. van de Walle. Free energy calculations of the mechanically unstable phases of PtTi and NiTi. *Acta Mater.*, 147:296, 2018. Download: [DOI] [Cite] .
- [33] A. van de Walle, S. Kadkhodaei, R. Sun, and Q.-J. Hong. Epicycle method for elasticity limit calculations. *Phys. Rev. B*, 95:144113, 2017. Download: [DOI] [Cite] [arXiv].
- [34] S. Kadkhodaei, Q.-J. Hong, and A. van de Walle. Free energy calculation of mechanically unstable but dynamically stabilized bcc titanium. *Phys. Rev. B*, 95:064101, 2017. Download: [DOI] [Cite] [arXiv] [Featured in Kaleidoscope].
- [35] A. van de Walle, Q.-J. Hong, S. Kadkhodaei, and R. Sun. The free energy of mechanically unstable phases. *Nature Commun.*, 6:7559, 2015. Download: [DOI] [Cite] .
- [36] J. Z. Liu, A. van de Walle, G. Ghosh, and M. D. Asta. Structure, energetics, and mechanical stability of Fe-Cu bcc alloys from first-principles calculations. *Phys. Rev. B*, 72:144109, 2005. Download: [DOI] [Cite] .
- [37] A. van de Walle, C. Tricot, and M. Gerspacher. Modeling carbon black reinforcement in rubber compound. *Kautschuk Gummi Kunststoffe*, 49:172, 1996. Download: [gzipped PS] [PDF].

## High-Temperature Materials

- [38] H. Liu, M. Asta, and A. van de Walle. Computational assessment of the efficacy of oxidation-resistant iridium coatings for multiple principal component rhenium substitutes. *Scripta Mater.*, 189:16, 2020. Download: [DOI] [Cite] .
- [39] S. V. Ushakov, A. Navrotsky, Q.-J. Hong, and A. van de Walle. Carbides and nitrides of zirconium and hafnium. *Materials*, 12:2728, 2019. Download: [DOI] [Cite] .
- [40] R. Sun, M. Asta, and A. van de Walle. First-principles thermal compatibility between Ru-based Re-substitute alloys and Ir coatings. *Comp. Mater. Sci.*, 170:109199, 2019. Download: [DOI] [Cite] .
- [41] Q.-J. Hong, S. V. Ushakov, D. Kapush, C. J. Benmore, R. J. K. Weber, A. van de Walle, and A. Navrotsky. Combined computational and experimental investigation of high temperature thermodynamics and structure of cubic ZrO<sub>2</sub> and HfO<sub>2</sub>. *Sci. Rep.*, 8:14962, 2018. Download: [DOI] [Cite] .
- [42] M. Fyhrrie, Q. Hong, D. Kapush, S.V. Ushakov, H. Liu, A. van de Walle, and A. Navrotsky. Energetics of melting of Yb<sub>2</sub>O<sub>3</sub> and Lu<sub>2</sub>O<sub>3</sub> from drop and catch calorimetry and first principles computations. *The Journal of Chemical Thermodynamics*, 132:405, 2019. Download: [DOI] [Cite] .
- [43] D. Kapush, S. V. Ushakov, A. Navrotsky, Q.-J. Hong, H. Liu, and A. van de Walle. A combined experimental and theoretical study of enthalpy of phase transition and fusion of yttria above 2000 °C using 'drop-n-catch' calorimetry and first-principles calculations. *Acta Mater.*, 124:204, 2017. Download: [DOI] [Cite] .
- [44] R. Chinnappan, B. K. Panigrahi, and A. van de Walle. First-principles study of phase equilibrium in Ti-V, Ti-Nb, and Ti-Ta alloys. *Calphad*, 54:125, 2016. Download: [DOI] [Cite] .

- [45] Q.-J. Hong and A. van de Walle. Prediction of the material with highest known melting point from ab initio molecular dynamics calculations. *Phys. Rev. B Rapid Communications*, 92:020104(R), 2015. Download: [DOI] [Cite] (Editor’s Suggestion). Featured in the Washington Post and on the Brown news site.
- [46] L. Miljacic, S. Demers, Q.-J. Hong, and A. van de Walle. Equation of state of solid, liquid and gaseous tantalum from first principles. *Calphad*, 51:133, 2015. Download: [DOI] [Cite] .
- [47] Q.-J. Hong, S. V. Ushakov, A. Navrotsky, and A. van de Walle. Combined computational and experimental investigation of the refractory properties of  $\text{La}_2\text{Zr}_2\text{O}_7$ . *Acta Mater.*, 84:275–282, 2015. Download: [DOI] [Cite] .
- [48] M. M. de Jong, D. L. Olmsted, A. van de Walle, and M. D. Asta. First-principles study of the structural and elastic properties of rhenium-based transition-metal alloys. *Phys. Rev. B*, 86:224101, 2012. Download: [DOI] [Cite] .
- [49] C. Ravi, B. K. Panigrahi, M. C. Valsakumar, and A. van de Walle. First-principles calculation of phase equilibrium of V-Nb, V-Ta, and Nb-Ta alloys. *Phys. Rev. B*, 85:054202, 2012. Download: [DOI] [Cite] .
- [50] B. P. Burton and A. van de Walle. First principles phase diagram calculations for the octahedral-interstitial system  $\text{HfO}_x$ ,  $0 \leq x \leq 1/2$ . *Calphad*, 37:151–157, 2012. Download: [DOI] [Cite] [arXiv].
- [51] B. P. Burton, A. van de Walle, and H. T. Stokes. First principles phase diagram calculations for the octahedral-interstitial system  $\text{ZrO}_X$ ,  $0 \leq X \leq 1/2$ . *J. Phys. Soc. Jpn.*, 81:014004, 2012. Download: [DOI] [Cite] [arXiv].
- [52] P. Dalach, D. E. Ellis, and A. van de Walle. First principles thermodynamic modeling of atomic ordering in yttria-stabilized zirconia. *Phys. Rev. B*, 82:144117, 2010. Download: [DOI] [Cite] .
- [53] 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. Download: [DOI] [Cite] .
- [54] O. Adjaoud, G. Steinle-Neumann, B.P. Burton, and A. van de Walle. First-principles phase diagram calculations for the  $\text{HfC-TiC}$ ,  $\text{ZrC-TiC}$ , and  $\text{HfC-ZrC}$  solid solutions. *Phys. Rev. B*, 80:134112, 2009. Download: [DOI] [Cite] .

## Energy Materials

- [55] G. S. Pomrehn, A. Zevalkink, A. van de Walle, and G. J. Snyder. Defect-driven properties in  $\text{AZn}_2\text{Sb}_2$  Zintl phases (A=Ca, Sr, Eu, Yb). *Angew. Chem. Int. Ed.*, 53, 2014. Download: [DOI] [Cite] .
- [56] S. Demers and A. van de Walle. Intrinsic defects and dopability of zinc phosphide. *Phys. Rev. B*, 85:195208, 2012. Download: [DOI] [Cite] .
- [57] B. G. Chirranjeevi and A. van de Walle. Ab initio thermodynamics of intrinsic oxygen vacancies in ceria. *Phys. Rev. B*, 86:134117, 2012. Download: [DOI] [Cite] [arXiv].
- [58] P. Dalach, D. E. Ellis, and A. van de Walle. First-principles thermodynamic modeling of lanthanum chromate perovskites. *Phys. Rev. B*, 85:014108, 2012. Download: [DOI] [Cite] .
- [59] G. S. Pomrehn, E. S. Toberer, G. J. Snyder, and A. van de Walle. Predicted electronic and thermodynamic properties of a newly discovered  $\text{Zn}_8\text{Sb}_7$  phase. *J. Am. Chem. Soc.*, 133:11255, 2011. Download: [DOI] [Cite] .
- [60] B. P. Burton, S. Demers, and A. van de Walle. First principles phase diagram calculations for the wurtzite-structure quasibinary systems  $\text{SiC-AlN}$ ,  $\text{SiC-GaN}$  and  $\text{SiC-InN}$ . *J. Appl. Phys.*, 110:023507, 2011. Download: [DOI] [Cite] .

- [61] G. S. Pomrehn, E. S. Toberer, G. J. Snyder, and A. van de Walle. Entropic stabilization and retrograde solubility in  $\text{Zn}_4\text{Sb}_3$ . *Phys. Rev. B*, 83:094106, 2011. Download: [DOI] [Cite] .
- [62] P. Tiwary, A. van de Walle, B. Jeon, and N. Gronbech-Jensen. Interatomic potentials for mixed oxide and advanced nuclear fuels. *Phys. Rev. B*, 83:094104, 2011. Download: [DOI] [Cite] [arXiv].
- [63] 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. Download: [DOI] [Cite] [arXiv].
- [64] R. Benedek, M. M. Thackeray, and A. van de Walle. Pourbaix-like phase diagram for lithium manganese spinels in acid. *J. Mat. Chem.*, 20:369, 2009. Download: [DOI] [Cite] .
- [65] R. Benedek and A. van de Walle. Reaction free energies of acid attack of lithium cobaltate. *Journal of the Electrochemical Society*, 155:A711, 2008. Download: [DOI] [Cite] .
- [66] R. Benedek, M. M. Thackeray, and A. van de Walle. Free energy for protonation reaction in lithium-ion battery cathode materials. *Chem. Mater.*, 20:5485, 2008. Download: [DOI] [Cite] .

## Interfaces

- [67] C. Nataraj, C. Woodward, and A. van de Walle. First-principles study of the effect of Al and Hf impurities on  $\text{Co}_3\text{W}$  antiphase boundary energies. *Acta Mater.*, submitted, 2021.
- [68] R. Sun, C. Woodward, and A. van de Walle. First-principles study on  $\text{Ni}_3\text{Al}$   $\{111\}$  antiphase boundaries with Ti and Hf impurities. *Phys. Rev. B*, 95:214121, 2017. Download: [DOI] [Cite] .
- [69] M. de Jong, L. Qi, D. L. Olmsted, A. van de Walle, and M. Asta. Calculations of planar defect energies in substitutional alloys using the special-quasirandom-structure approach. *Phys. Rev. B*, 93:094101, 2016. Download: [DOI] [Cite] .
- [70] R. Sun and A. van de Walle. Automating impurity-enhanced antiphase boundary energy calculations from ab initio monte carlo. *Calphad*, 53:20, 2016. Download: [DOI] [Cite] .
- [71] M. M. de Jong, J. Kacher, M.H.F. Sluiter, L. Qi, D.L. Olmsted, A. van de Walle, J. W. Morris, A.M. Minor, and M. D. Asta. Electronic origins of anomalous twinning in hexagonal close packed transition metals. *Phys. Rev. Lett.*, 115:065501, 2015. Download: [DOI] [Cite] Featured on the cover.
- [72] C. Woodward, A. van de Walle, M. D. Asta, and D. Trinkle. First-principles study of interfacial boundaries in  $\text{Ni-Ni}_3\text{Al}$ . *Acta Mater.*, 75:60–70, 2014. Download: [DOI] [Cite] .
- [73] A. van de Walle, B. G. Chirranjeevi, S. Demers, Q.-J. Hong, A. Kowalski, L. Miljacic, G. S. Pomrehn, and P. Tiwary. Ab initio calculation of anisotropic interfacial excess free energies. *Phys. Rev. B*, 89:184101, 2014. Download: [DOI] [Cite] [arXiv] [Featured in Kaleidoscope].
- [74] R. V. Chepulskii, W. H. Butler, A. van de Walle, and S. Curtarolo. Surface segregation in nanoparticles from first principles: The case of  $\text{FePt}$ . *Scripta Materialia*, 62:179, 2010. Download: [DOI] [Cite] [arXiv].
- [75] 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. Download: [DOI] [Cite] .
- [76] C. H. Lanier, A. van de Walle, N. Erdman, E. Landree, O. Warschkow, A. Kazimirov, K. R. Poepelmeier, J. Zegenhagen, M. D. Asta, and L. D. Marks. The  $c(6 \times 2)$  reconstruction on the  $\text{SrTiO}_3$  (001) surface. *Phys. Rev. B*, 76:045421, 2007. Download: [DOI] [Cite] [arXiv].
- [77] M. J. Beck, A. van de Walle, and M. D. Asta. Surface energetics and structure of the Ge wetting layer on Si (100). *Phys. Rev. B*, 70:205337, 2004. Download: [DOI] [Cite] [from PRB online].

- [78] A. van de Walle, M. D. 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. Download: [DOI] [Cite] [arXiv] [from PRB online].
- [79] A. van de Walle and M. D. 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. Download: [DOI] [Cite] [arXiv] [from Science Direct].
- [80] H. Ramalingam, M. D. 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. Download: [DOI] [Cite] .

## Density Functional Theory

- [81] H. Chen, Q.-J. Hong, S. Ushakov, A. Navrotsky, and A. van de Walle. A simple method for computing the formation energies of metal oxides. *Comput. Mat. Sci.*, in preparation, 2021.
- [82] Q.-J. Hong, J. Yasi, and A. van de Walle. A tetrahedron-tiling method for crystal structure prediction. *Phys. Rev. Materials Rapid Communications*, 1:020801(R), 2017. Download: [DOI] [Cite] [arXiv].
- [83] B. Meredig, A. Thompson, H.A. Hansen, C. Wolverton, and A. van de Walle. A method for locating low-energy solutions within DFT+U. *Phys. Rev. B*, 82:195128, 2010. Download: [DOI] [Cite] .
- [84] A. van de Walle and G. Ceder. Correcting overbinding in LDA calculations. *Phys. Rev. B*, 59:14992, 1999. Download: [DOI] [Cite] .

## Alloy Thermodynamics

- [85] 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*, accepted, 2020.
- [86] 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*, 34:113, 2010. Download: [DOI] [Cite] .
- [87] A. van de Walle. First-principles alloy thermodynamics. In P. Derosa and T. Cagin, editors, *Multiscale Modeling: From Atoms to Devices*. CRC press, 2010.
- [88] G. Ghosh, A. van de Walle, and M. D. 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. Download: [DOI] [Cite] .
- [89] 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. Download: [DOI] [Cite] [arXiv] [from PRB online].
- [90] G. Ghosh, A. van de Walle, and M. D. Asta. First-principles phase stability calculations of pseudobinary alloys of  $(\text{Al,Zn})_3\text{Ti}$  with  $\text{L}_{12}$ ,  $\text{DO}_{22}$  and  $\text{DO}_{23}$  structures. *J. Phase Equilib. Diff.*, 28:9, 2007. Download: [DOI] [Cite] [PDF].
- [91] 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. Download: [DOI] [Cite] .
- [92] 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. Download: [DOI] [Cite] .

- [93] R. Arroyave, A. van de Walle, and Z.-K. Liu. First-principles calculations of the Zn-Zr system. *Acta Mater.*, 54:473, 2006. Download: [DOI] [Cite] .
- [94] A. van de Walle. Genesis of crystal structures (in “news and views”). *Nat. Mater.*, 4:362, 2005. Download: [DOI] [Cite] .
- [95] A. van de Walle, G. Ghosh, and M. D. 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. Download: [DOI] [Cite] .
- [96] A. van de Walle and M. D. Asta. First-principles modeling of phase equilibria. In S. Yip, editor, *Handbook of Materials Modeling*, volume Part A. Springer, Dordrecht, the Netherlands, 2005. Download: [DOI] [Cite] [From Springer].
- [97] R. Benedek, A. van de Walle, S. Gerstl, M. D. Asta, D. N. Seidman, and C. Woodward. Partitioning of solutes in multiphase TiAl alloys. *Phys. Rev. B*, 71:094201, 2005. Download: [DOI] [Cite] [from PRB online].
- [98] A. van de Walle, Z. Moser, and W. Gasior. First-principles calculation of the Cu-Li phase diagram. *Arch. Metall. Mater.*, 49:535, 2004. Download: [PDF] [Caltech].
- [99] D. Morgan, B. Wang, G. Ceder, and A. van de Walle. First-principles study of magnetism in spinel  $\text{MnO}_2$ . *Phys. Rev. B*, 67:134404, 2003. Download: [DOI] [Cite] [From PRB online].
- [100] D. Balachandran, D. Morgan, G. Ceder, and A. van de Walle. First-principles study of the structure of stoichiometric and Mn-deficient  $\text{MnO}_2$ . *J. of Solid State Chem.*, 173:462, 2003. Download: [DOI] [Cite] .
- [101] D. Morgan, D. Balachandran, G. Ceder, and A. van de Walle. A drastic influence of point defects on phase stability in  $\text{MnO}_2$ . In M. Greenblatt, M.A. Alario-Franco, M.S. Whittingham, and G. Rohrer, editors, *MRS Proceedings*, volume 755, pages DD2.8–1, 2002. Download: [DOI] [Cite] [From MRS site].

## Phonons

- [102] J. Z. Liu, G. Ghosh, A. van de Walle, and M. D. 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. Download: [DOI] [Cite] .
- [103] B.P. Burton and A. van de Walle. First principles phase diagram calculations for the system NaCl-KCl: the role of excess vibrational entropy. *Chem. Geol.*, 225:222, 2006. Download: [DOI] [Cite] .
- [104] 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. Download: [DOI] [Cite] [arXiv].
- [105] 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. *Phys. Chem. Miner.*, 30:88, 2003. Download: [DOI] [Cite] .
- [106] A. van de Walle and G. Ceder. The effect of lattice vibrations on substitutional alloy thermodynamics. *Rev. Mod. Phys.*, 74:11–45, 2002. Download: [DOI] [Cite] [arXiv] [errata].
- [107] A. van de Walle and G. Ceder. First-principles computation of the vibrational entropy of ordered and disordered  $\text{Pd}_3\text{V}$ . *Phys. Rev. B*, 61:5972, 2000. Download: [DOI] [Cite] [arXiv].
- [108] 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. Download: [DOI] [Cite] [PDF].
- [109] A. van de Walle, G. Ceder, and U. V. Waghmare. First-principles computation of the vibrational entropy of ordered and disordered  $\text{Ni}_3\text{Al}$ . *Phys. Rev. Lett.*, 80:4911, 1998. Download: [DOI] [Cite] [arXiv].

## Glasses

- [110] R. Ojeda Mota, E. Lund, S. Sohn, D. Browne, D. Hofmann, S. Curtarolo, A. Van de Walle, and J. Schroers. Enhancing ductility in bulk metallic glasses by straining during cooling. *Communications Materials*, accepted, 2021.