Christopher Wolverton
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Northwestern University
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The Open Quantum Materials Database (http://oqmd.org)

PROFESSIONAL PREPARATION

1983-1987 B. S. in Physics, **The University of Texas at Austin** (*Summa cum laude*)
1987-1993 Ph.D in Physics, **University of California at Berkeley**
1993-1996 Postdoctoral Research Associate, **National Renewable Energy Lab.**

APPOINTMENTS

2007-pres. Professor, **Northwestern University**
2004-2006 Technical Leader, **Ford Research Laboratory**, Dearborn, MI.
Group Leader: Hydrogen Storage and Nanoscale Modeling Group
1999-2003 Senior Technical Specialist, **Ford Research Laboratory**, Dearborn, MI.
1996-1999 Staff Scientist, **National Renewable Energy Lab.**, Golden, CO.

AWARDS

JOM Best Paper Award, Structural Metals Division, 2014
Walder Award for Research Excellence, Northwestern University, 2013
Fellow, American Physical Society, 2011.
Ford Motor Company Technical Achievement Award, 2006.
USCAR Recognition Award, 2006.
Noah Greenberg Award, American Musicological Society, 2006.
Ford Motor Company Patent Award, 2005.
Ford Motor Company Publication Award, 2005.
Ford Environmental, Physical Sciences, and Safety Research Recognition Award, 2003.
John E. Dorn Memorial Lecture, Northwestern University, 2003.
Ford Motor Company Patent Award, 2002.

>250 peer-reviewed publications / >200 Invited talks / 9 patents granted (several more pending); ~15000 total citations; **h-index of 67 (Google Scholar)**; (see attached list of publications/invited talks/patents)

EXTERNAL SERVICE/PROFESSIONAL SOCIETY ACTIVITIES

Committees
Editorial Board, *Scientific Data*
Editorial Board, *npj Computational Materials*
Advisory Board, NCCR MARVEL Center, Switzerland, 2015-present
DOE Workshop on Exascale Computing, Discussion Leader, 2015
Advisory Board, Citrine Informatics, 2014-present

APS McGroddy Prize for New Materials Selection Committee, 2014-2016
MRS Materials Theory Award Committee, 2011-2014
TMS Fellowship Committee, 2011-2014
TMS Integrated Computational Materials Engineering Committee, 2009-present.
TMS Alloy Phases Committee, 2006-present.
TMS Computational Materials Science Committee, 2006-present.
MRS Energy Quarterly Guest Editor, 2011
Member, International Commission C20 of IUPAP on Computational Physics, 2006-2011.
TMS Integrated Computational Materials Engineering Task Force, 2006-2009.
Guest Editor, MRS Bulletin, Sept. 2006.
Member, DOE/FreedomCAR Hydrogen Storage Technical Team, 2003-2006.
Invited Participant - National Academy of Engineering, Frontiers of Engineering workshop, 2006.
TMS Advisory Board, 2003-2004.

Conferences, Workshops, Symposia Organized

Organizer, TMS Annual Meeting, "Computational Thermodynamics and Kinetics", Nashville, 2016.
Organizer, TMS Annual Meeting, Hume-Rothery Symposium "Electronic Structure Theory of Stability and Bonding in Alloys", San Antonio, 2013.
Organizer, Fall MRS Meeting Symposium, "Advanced Multiscale Materials Simulation–Toward Inverse Materials Computation", Boston, MA 2012.
Organizer, TMS Annual Meeting, Hume-Rothery Symposium "Configurational Thermodynamics of Materials", Seattle, WA, 2010.
Organizer, International Materials Research Congress, Symposium, "Theory and Computer Simulation of Materials", Cancun, Mexico, 2009.
Organizer, DOE Workshop on Theory and Simulation of Hydrogen Storage Materials, 2008.
Organizer, 2007 TMS MS&T Meeting, Symposium, "High-Density Hydrogen Storage for Automotive Applications"
Organizer, 2007 ACS Spring Meeting, Symposium, "Capturing Complexity in Physical Sciences Simulation"
Organizer, International Workshop, "Theory Meets Industry", Vienna, 2007.
Organizer, 2006 APS March Meeting, Symposium, "Catalysis and Complexity: Ken Hass Memorial"
Organizer, DOE Workshop on Theory and Simulation of Hydrogen Storage Materials, 2006.
Organizer, 2004 APS March Meeting, Symposium, "Perspectives on Hydrogen Storage"
Organizer, 2001 APS March Meeting, Symposium, "Materials Theory and Computation for Industrial Problems"
Organizer, International Workshop, "Thermodynamics and Structural Properties of Alloy Materials", Aruba, 1999.

Review Activities

Reviewer for many journals, e.g., Science, Nature, Nature Materials, Nature Reviews, Phys. Rev. Lett., Acta Mater., J. Amer. Chem. Soc, etc.
Reviewer for many funding agencies, e.g., NSF, DOE-BES, DOE-EERE.

NORTHWESTERN SERVICE ACTIVITIES

Data Science Initiative, Seed Award Review Committee, 2015-present

Co-Director, Integrated Computational Materials Engineering (ICME) Masters Certificate, 2011-present
Director, MSE Graduate Admissions, 2011-2014
MSE Graduate Admissions Committee, 2010-2014, 2016-present
Undergraduate Advisor, 2007-2015
McCormick Computing Committee, 2007-2015
Office of Research Integrity, Scientific Misconduct Committee, 2011-2013
Visit to Shanghai Jiao Tong University to initiate/propose collaborative Masters program, 2011, 2012
Applied Physics Program Recruiting Committee, 2010
MSE Graduate Curriculum Committee, 2008-2011
MSE Undergraduate Curriculum Committee, 2008-2011
McCormick "Energy Strategy" Committee: Responsible for forming and launching the Center for Energy Efficient Transportation (CEET), 2007
Organizer, Domain Dinner on Energy Efficient Transportation, Dec. 2007
Chair, MSE Computing Committee, 2007-2011
Organizer, NU Symposium on Atomic-Scale Modeling, July 2007

Graduate Students and Postdoctoral Associates:

Former Graduate Students (PhD) (13):
Wei Chen (IIT), Bryce Meredig (Citrine Informatics), Alex Thompson, Yongli Wang, Scott Kirklin, Ahmed Issa, Jeff Doak (Questek), Murat Aykol (Toyota Research), Kyoungdoc Kim (Northwestern), Logan Ward (U. Chicago), David Snydacker (Lilac Solutions), Tony Emery (Solvay), Soo Kim (MIT)

Former Graduate Students (MS) (7):
Danny Shapiro, Yue Li, Dongshu Wang, Quan Xiu, Zhe Luo, Qing Dong, Yishan Shi

Current Graduate Students (13 PhD, 1MS):
Zhi Lu, Zhenpeng Yao, Vinay Hedge, Mohan Liu, Jonathan Pfluger, Shane Patel, Xia Hua, Eric Schwenker, Cheol Peter Park, Sean Griesemer, Abhijith Gopakumar, Jiahong Shen, Bianca Baldassarri, Chonghao Peng

Former Postdocs (12):
Dongwon Shin (ORNL), Dilpuneet Aihdy (U. Wyoming), William Art Counts (Apple), Swetha Ganeshan, David Farrell (Ford), Heine Hansen (Technical Univ. of Denmark), Zugang Mao, Yongsheng Zhang (Institute of Solid State Physics, Chinese Academy of Sciences), James Saal (Questek), Jishnu Bhattacharya (IIT Kharagpur), Kyle Michel (Citrine Informatics), Vancho Kocevski (U. South Carolina)

Current Postdocs (7):
Shiqiang Hao, Shahab Naghavi, Max Amsler, Jiangang He, Eric Isaacs, Bi-Cheng Zhao, Koushik Pal (starting Nov. 1, 2017)

Undergraduate Students Supervised:
Wenhao Sun, Michelle Chen, Jihye Park, Sail Wu, Scott Grindy, Julija Vinckeviciute, Yang Yu, Kareem Youseff, Kyle Bushick

PUBLICATIONS/PATENTS/AWARDS

Prof. Christopher Wolverton – REFEREED PUBLICATIONS

2017

264. J. Zhao, S. M. Islam, S. Hao, G. Tan, X. Su, H. Chen, W. Lin, R. Li, C. Wolverton, and M. G. Kanatzidis, "*Semiconducting Pavonites CdMBi4Se8 (M= Sn and Pb) and Their Thermoelectric Properties*", Chem. Mater. **29**, 8494 (2017). DOI: 10.1021/acs.chemmater.7b03328

263. Z. Yao, S. Kim, M. Aykol, Q. Li, J. Wu, J. He, and C. Wolverton, "*Revealing the Conversion Mechanism of Transition Metal Oxide Electrodes during Lithiation from First Principles*", Chem. Mater. **29**, 9011 (2017). DOI: 10.1021/acs.chemmater.7b02058

262. V. Kocevski and C. Wolverton, "*Designing high-efficiency nanostructured two-phase Heusler thermoelectrics*", Chem. Mater. **29**, 9386 (2017). DOI: 10.1021/acs.chemmater.7b03379

261. D. H. Snydacker, V. I. Hegde, and C. Wolverton, "*Electrochemically Stable Coating Materials for Li, Na, and Mg Metal Anodes in Durable High Energy Batteries*", J. Electrochem. Soc. **164**, A3582 (2017).

260. A. M. Jokisaari, S. S. Naghavi, C. Wolverton, P. W. Voorhees and O. G. Heinonen, "*Predicting the morphologies of γ' precipitates in cobalt-based superalloys*", Acta Mater. **141**, 273 (2017).

259. K. Kim, A. Roy, M. P. Gururajan, C. Wolverton and P. W. Voorhees, "*First-principles/Phase-field modeling of θ' precipitation in Al-Cu alloys*", Acta Mater. **140**, 344 (2017).

258. A. A. Emery and C. Wolverton, "*High-throughput DFT calculations of formation energy, stability and oxygen vacancy formation energy of ABO_3 perovskites*", Sci. Data **4**, 170153 (2017).

257. K. He, Z. Yao, S. Hwang, N. Li, K. Sun, H. Gan, Y. Du, H. Zhang, C. Wolverton, and D. Su, "*Kinetically-Driven Phase Transformation during Lithiation in Copper Sulfide Nanoflakes*", Nano Lett. **17**, 5726 (2017).

256. M. Amsler and C. Wolverton, "*Dense superconducting phases of copper-bismuth at high pressure*", Phys. Rev. Materials **1**, 031801(R) (2017).

255. S. Kim, M. Aykol, V. I. Hegde, Z. Lu, S. Kirklin, J. R. Croy, M. M. Thackeray, and C. Wolverton, "*Materials Design of High-Capacity Li-rich Layered-Oxide Electrodes: Li_2MnO_3 and Beyond*" Energy Env. Sci. **10**, 2201 (2017).

254. A. Bobel, K. Kim, C. Wolverton, M. Walker, and G. B. Olson, "*Equilibrium composition variation of Q-phase precipitates in aluminum alloys*", Acta Mater. **138**, 150 (2017). DOI: 10.1016/j.actamat.2017.07.048

253. J. Zhao, S. M. Islam, S. Q. Hao, G. J. Tan, C. C. Stoumpos, C. Wolverton, H. J. Chen, Z. Z. Luo, R. K. Li, and M. G. Kanatzidis, "*Homologous Series of 2D Chalcogenides Cs-Ag-Bi-Q (Q = S, Se) with Ion-Exchange Properties*", J. Amer. Chem. Soc. **139**, 12601 (2017). DOI: 10.1021/jacs.7b06373

252. S. S. Naghavi, A. A. Emery, H. A. Hansen, F. Zhou, V. Ozolins and C. Wolverton, "*Giant onsite electronic entropy enhances the performance of ceria for water splitting*", Nat. Commun. **8**, 285 (2017).

251. Q. Q. Li, Z. P. Yao, J. S. Wu, S. Mitra, S. Q. Hao, T. S. Sahu, Y. Li, C. Wolverton, V. P. Dravid, "*Intermediate phases in sodium intercalation into MoS_2 nanosheets and their implications for sodium-ion batteries*", Nano Energy **38**, 342 (2017). DOI: 10.1016/j.nanoen.2017.05.055

250. L. Ward, R. Liu, A. Krishna, V. Hegde, A. Agrawal, A. Choudhary, and C. Wolverton., "*Including crystal structure attributes in machine learning models of formation energies via Voronoi tessellations*", Phys. Rev. B **96**, 024104 (2017).

249. M. Aykol, J. W. Doak, and C. Wolverton, "*Phosphorus Allotropes: Stability of Black versus Red*" Phys. Rev. B **95** 214115 (2017).

248. S. M. Clarke, M. Amsler, J. P. S. Walsh, T. Yu, Y. B. Wang, Y. Meng, S. D. Jacobsen, C. Wolverton, and D. E. Freedman, "*Creating Binary Cu-Bi Compounds via High-Pressure Synthesis: A Combined Experimental and Theoretical Study*", Chem. Mater. **29**, 5276 (2017). DOI: 10.1021/acs.chemmater.7b01418

247. S. S. Naghavi, V. I. Hegde, C. Wolverton, "*Diffusion coefficients of transition metals in fcc cobalt*", Acta Mater. **132**, 467 (2017).

246. L. Ward, C. Wolverton, "*Atomistic calculations and materials informatics: A review*", Curr. Opin. Solid State Mater. Sci. **21**, 167 (2017).

245. S. Ohno, U. Aydemir, M. Amsler, J. H. Pohls, S. Chanakian, A. Zevalkink, M. A. White, S. K. Bux, C. Wolverton, and G. J. Snyder, "*Achieving zT > 1 in Inexpensive Zintl Phase $Ca_9Zn_{4+x}Sb_9$ by Phase Boundary Mapping*", Adv. Funct. Mater. **27**, 1606361 (2017). DOI: 10.1002/adfm.201606361

244. G. Tan, S. Hao, J. Zhao, C. Wolverton, and M. Kanatzidis, "*High Thermoelectric Performance in Electron-doped AgBi3S5 with Ultralow Thermal Conductivity*", J. Amer. Chem. Soc. **139**, 6467 (2017).

243. E. D. Hanson, L. Lajaunie, S. Hao, B. D. Myers, F. Shi, A. A. Murthy, C. Wolverton, R. Arenal, and V. P. Dravid, "*Systematic Study of Oxygen Vacancy Tunable Transport Properties of Few-Layer MoO_{3-x} Enabled by Vapor-Based Synthesis*", Adv. Funct. Mater. **27**, 1605380 (2017).

242. K. S. Chen, R. Xu, N. S. Luu, E. B. Secor, K. Hamamoto, Q. Q. Li, S. Kim, V. K. Sangwan, I. Balla, L. M. Guiney, J. W. T. Seo, X. K. Yu, W. W. Liu, J. S. Wu, C. Wolverton, V. P. Dravid, S. A. Barnett, J. Lu, K. Amine, and M. C. Hersam, "*Comprehensive Enhancement of Nanostructured Lithium-Ion Battery Cathode Materials via Conformal Graphene Dispersion*", Nano Lett. **17**, 2539 (2017). DOI: 10.1021/acs.nanolett.7b00274

241. J. G. He, S. Q. Hao, Y. Xia, S. S. Naghavi, V. Ozolins, and C. Wolverton, "*Bi_2PdO_4: A Promising Thermoelectric Oxide with High Power Factor and Low Lattice Thermal Conductivity*", Chem. Mater. **29** 2529 (2017). DOI: 10.1021/acs.chemmater.6b04230

240. J. Zhao, S. M. Islam, G. J. Tan, S. Q. Hao, C. Wolverton, R. K. Li, and M. G. Kanatzidis, "*The New Semiconductor $Cs_4Cu_3Bi_9S_{17}$*", Chem. Mater. **29**, 1744 (2017). DOI: 10.1021/acs.chemmater.6b05298

239. H. Bin, Z. Yao, S. Zhu, C. Zhu, H. Pan, Z. Chen, C. Wolverton, and D. Zhang, "*A high-performance anode material based on FeMnO 3/graphene composite*", J. Alloys Comp. **695**, 1223 (2017).

238. W. G. Zeier, S. Anand, L. Huang, R. He, H. Zhang, Z. Ren, C. Wolverton, and G. J. Snyder, "*Using the 18-Electron Rule To Understand the Nominal 19-Electron Half-Heusler NbCoSb with Nb Vacancies*", Chem. Mater. **29**, 1210 (2017). DOI: 10.1021/acs.chemmater.6b04583

237. S. Xu, R. Jacobs, C. Wolverton, T. Kuech, and D. Morgan, "*Nanoscale Voltage Enhancement at Cathode Interfaces in Li-ion Batteries*", Chem. Mater. **29**, 1218 (2017).

236. S. S. Naghavi, V. I. Hegde, A. Saboo, and C. Wolverton, "*Energetics of cobalt alloys and compounds and solute–vacancy binding in fcc cobalt: A first-principles database*", Acta Mater. **124**, 1 (2017).

235. L. W. Hart, L. J. Nelson, R. R. Vanfleet, B. J. Campbell, M. H. F. Sluiter, J. H. Neethling, E. J. Olivier, S. Allies, C. I. Lang, B. Meredig, and C. Wolverton, "*Revisiting the revised Ag-Pt phase diagram*", Acta Mater. **124**, 325 (2017).

234. J. Ma, V. I. Hegde, K. Munira, Y. Xie, S. Keshavarz, D. T. Mildebrath, C. Wolverton, A. W. Ghosh, and W. H. Butler, "*Computational investigation of half-Heusler compounds for spintronics applications*", Phys. Rev. B **95**, 024411 (2017).

233. D. Snydacker and C. Wolverton, "*Oxygen evolution from olivine $Mn_{1-x}M_xPO_4$ (M=Fe, Ni, Al, Mg) delithiated cathode materials*", Phys. Rev. B **95**, 024102 (2017).

232. M. Amsler, S. S. Naghavi, and C. Wolverton, "*Prediction of superconducting iron-bismuth intermetallic compounds at high pressure*", Chem. Sci. **8**, 2226 (2017).

231. L. Nguyen, L. Liu, S. Assefa, C. Wolverton, W. F. Schneider, and .F. F. Tao, "*Atomic-Scale Structural Evolution of Rh(110) during Catalysis*", ACS Catal. **7**, 664 (2017).

2016

230. M. Aykol, S. Kim, V. I. Hegde, D. Snydacker, Z. Lu, S. Hao, S. Kirklin, D. Morgan, and C. Wolverton, "*High-throughput Computational Design of Cathode Coatings for Lithium-ion Batteries*", Nature Commun. **7**, 13779.(2016).

229. Y. Li, J. D Cain, E. D Hanson, A. A. Murthy, S. Hao, F. Shi, Q. Li, C. Wolverton, X. Chen, V. P. Dravid, "*Au@ MoS_2 Core-shell Heterostructures with Strong Light-Matter Interactions*", Nano Lett. **16**, 7696 (2016).

228. D. H. Snydacker, M. Aykol, S. Kirklin, and C. Wolverton, "*Lithium-Ion Cathode/Coating Pairs for Transition Metal Containment*", J. Electrochem. Soc. **163**, A2054 (2016).

227. Ward, A. Agrawal, A. Choudhary, and C. Wolverton., "*A General-Purpose Machine Learning Framework for Predicting Properties of Inorganic Materials*" npj Computational Materials **2**, 16028 (2016).

226. S. Hao, V. P. Dravid, M. G. Kanatzidis, and C. Wolverton, "*Prediction of high figure of merit plateau in SnS and solid solution of (Pb,Sn)S*", APL Mater. **4**, 104505 (2016).

225. L.-D. Zhao, S.-H. Lo, Y. Zhang, H. Sun, G. Tan, C. Uher, C. Wolverton, V. P. Dravid, and M. G Kanatzidis, "*The intrinsic thermal conductivity of SnSe: Reply*", Nature **539**, 7627 (2016).

224. E. Lee, J. Blauwkamp, F. C. Castro, J. Wu, V. P. Dravid, P. Yan, C. Wang, S. Kim, C. Wolverton, R. Benedek, F. Dogan, J. Sun Park, J. R. Croy, and M. M. Thackeray, "*Exploring Lithium-Cobalt-Nickel Oxide Spinel Electrodes for ≥3.5 V Li-Ion Cells*", ACS Appl. Mater. Interfaces, **8**, 27720 (2016).

223. S. M. Clarke, J. P. S. Walsh, M. Amsler, C. D. Malliakas, T. Yu, S. Goedecker, Y. Wang, C. Wolverton, and D. E. Freedman, "*Discovery of a Superconducting Cu–Bi Intermetallic Compound by High-Pressure Synthesis*", Angew.Chem. Int. Ed. **55**,13446 (2016).

222. H. Lin, G. Tan, J.-N. Shen, S. Hao, L.-M. Wu, N. Calta, C. Malliakas, S. Wang, C. Uher, C. Wolverton, and M. G. Kanatzidis, "*Concerted Rattling in $CsAg_5Te_3$ Leading to Ultralow Thermal Conductivity and High Thermoelectric Performance*", Angew.Chem. Int. Ed.**55**, 11431 (2016).

221. Q. Li, H. Liu, Z. Yao, J. Cheng, T. Li, Y. Li, C. Wolverton, J. Wu, and V. P. Dravid, "*Electrochemistry of Selenium with Sodium and Lithium: Kinetics and Reaction Mechanism*", ACS Nano **10** , 8788 (2016).

220. Y. S. Gim, Y. Lee, S. Kim, S. Hao, M. S. Kang, W. J. Yoo, H. Kim, C. Wolverton, and J. H. Cho, "*Organic Dye Graphene Hybrid Structures with Spectral Color Selectivity*", Adv. Funct. Mater. **26**, 6593 (2016).

219. A. A. Emery, J. E. Saal, S. Kirklin, V. I. Hegde, and C. Wolverton, "*High-Throughput Computational Screening of Perovskites for Thermochemical Water Splitting Applications*" Chem. Mater. **28**, 5621 (2016).

218. Y. Zhang, S. Hao, L.-D. Zhao, C. Wolverton and Z. Zeng, "*Pressure induced thermoelectric enhancement in SnSe crystals*", J. Mater. Chem. A **4**, 12073 (2016).

217. J. He, M. Amsler, Y. Xia, S. S. Naghavi, V. I. Hegde, S. Hao, S. Goedecker, V. Ozoliņš, and C. Wolverton, "*Ultralow Thermal Conductivity in Full Heusler Semiconductors*", Phys. Rev. Lett. **117**, 046602 (2016).

216. S. Hao, Z. Lu, and C. Wolverton, "*Quaternary Phase Diagrams of $Li_yVa_{1-y}Mn_xNi_{2-x}O_4$ and Composite Cathode Voltages from First-Principles*", Phys. Rev. B **94**, 014114 (2016).

215. G. Tan, F. Shi, S. Hao, L.-D. Zhao, H. Chi, X. Zhang, C. Uher, C. Wolverton, V. P. Dravid, and M. G. Kanatzidis, "*Non-equilibrium processing leads to record high thermoelectric figure of merit in PbTe–SrTe*", Nature Commun. **7**, 12167 (2016).

214. M. Amsler, S. Goedecker, W. G. Zeier, G. J. Snyder C. Wolverton, and L. Chaput , "*ZnSb polymorphs with improved thermoelectric properties*", Chem. Mater. **28**, 2912 (2016).

213. S. Hao, F. Shi, V. P. Dravid, M. G. Kanatzidis, and C. Wolverton, "*Computational Prediction of High Thermoelectric Performance in Hole Doped Layered GeSe*", Chem. Mater **28**, 3218 (2016).

212. J. Hill, G. Mulholland, K. Persson, R. Seshadri , C. Wolverton , and B. Meredig, "*Materials science with large-scale data and informatics: Unlocking new opportunities*", MRS Bulletin **41**, 399 (2016).

211. Y. Wang, K. Michel, and C. Wolverton, "*Hydrogen diffusion in bulk MgB_2*", Scripta Mater. **117**, 86 (2016).

210. N. Naghibolashrafi, S. Keshavarz, V. I. Hegde, A. Gupta, W. H. Butler, J. Romero, K. Munira, P. LeClair, D. Mazumdar, J. Ma, A. W. Ghosh, and C. Wolverton, "*Synthesis and characterization of Fe-Ti-Sb intermetallic compounds: Discovery of a new Slater-Pauling phase*", Phys. Rev. B **93**, 104424 (2016).

209. D. H. Snydacker and C. Wolverton, "Transition-Metal Mixing and Redox Potentials in $Li_x(M_{1-y}M'_y)PO_4$ (M, M′ = Mn, Fe, Ni) Olivine Materials from First-Principles Calculations", J. Phys. Chem. C **120**, 5932 (2016).

208. A. M. Deml, R. O'Hayre, C. Wolverton, and V. Stevanović, "*Predicting density functional theory total energies and enthalpies of formation of metal-nonmetal compounds by linear regression*", Phys. Rev. B **93**, 085142 (2016).

207. Z. Mao, D. N. Seidman, and C. Wolverton, "*Erratum: 'The effect of vibrational entropy on the solubility and stability of ordered Al3Li phases in Al–Li alloys' [APL Mater. 1, 042103 (2013)]*", APL Mater. **4**, 029901 (2016).

206. J. A. Flores-Livas, M. Amsler, C. Heil, A. Sanna, L. Boeri, G. Profeta, C. Wolverton, S. Goedecker, and E. K. U. Gross, "*Superconductivity in metastable phases of phosphorus-hydride compounds under high pressure*" Phys. Rev. B **93**, 020508(R) (2016).

205. L. Zhu, M. Amsler, T. Fuhrer, B. Schaefer, S. Faraji, S. Rostami, S. Alireza Ghasemi, A. Sadeghi, M. Grauzinyte, C. Wolverton, and S. Goedecker, "*A fingerprint based metric for measuring similarities of crystalline structures*" J. Chem. Phys. **144**, 034203 (2016).

204. J. E. Saal and C. Wolverton, "Energetics of antiphase boundaries in γ′ Co3(Al,W)-based superalloys", Acta Materialia **103**, 57 (2016).

203. S. Kim, J.-K. Noh, M. Aykol, Z. Lu, H. Kim, W. Choi, C. Kim, K. Yoon Chung, C. Wolverton, and B.-W. Cho, "*Layered-Layered-Spinel Cathode Materials Prepared by a High-Energy Ball-Milling Process for Lithium-ion Batteries*", ACS Appl. Mater. Interfaces **8**, 363 (2016).

202. L. D. Zhao, G. Tan, S. Hao, J. He, Y. Pei, H. Chi, H. Wang, S. Gong, H. Xu, V. P. Dravid, C. Uher, G. J. Snyder, C. Wolverton, and M. G. Kanatzidis, "*Ultrahigh power factor and thermoelectric performance in hole-doped single-crystal SnSe*", Science **351**, 141 (2016).

201. S. Bajaj, H. Wang, J. W. Doak, C. Wolverton and G. J. Snyder, "*Calculation of dopant solubilities and phase diagrams of X–Pb–Se (X = Br, Na) limited to defects with localized charge*", J. Mater. Chem. C **4**, 1769 (2016).

200. A. K. Kercher, J. A. Kolopus, K. J. Carroll, R. R. Unocic, S. Kirklin, C.Wolverton, S. L. Stooksbury, L. A. Boatner, and N. J. Dudney, "*Mixed Polyanion Glass Cathodes: Glass-State Conversion Reactions*", J. Electrochem. Soc. 163, **A131** (2016).

199. S. Kirklin, J. E. Saal, V. I. Hegde, and C. Wolverton, "*High-throughput computational search for strengthening precipitates in alloys*" Acta Materialia **102**, 125 (2016).

2015

198. J. W. Doak, C. Wolverton, and V. Ozolins, "*Vibrational contributions to the phase stability of PbS-PbTe alloys*", Phys. Rev. B **92**, 174306 (2015).

197. S. Kirklin, J. Saal, B. Meredig, A. Thompson, J. Doak, M. Aykol, S. Ruhl, and C. Wolverton, "*The Open Quantum Materials Database (OQMD): Assessing the Accuracy of DFT Formation Energies*", npj Computational Materials **1**, 15010 (2015).

196. Y. Yu, M. Aykol, and C. Wolverton, "*Reaction thermochemistry of metal sulfides with GGA and GGA+ U calculations*", Phys. Rev. B **92**, 195118 (2015).

195. S. Kim, M. Aykol, and C. Wolverton, "*Surface phase diagram and stability of (001) and (111) LiMn2O4 spinel oxides*", Phys. Rev. B **92**, 115411 (2015).

194. L. Jaber-Ansari, K. P. Puntambekar, S. Kim, M. Aykol, L. L. Luo, J. S. Wu, B. D. Myers, H. Iddir, J. T. Russell, S. J. Saldana, R. Kumar, M. M. Thackeray, L. A. Curtiss, V. P. Dravid, C. Wolverton, and M. C. Hersam, "*Suppressing Manganese Dissolution from Lithium Manganese Oxide Spinel Cathodes with Single-Layer Graphene*", Adv. Energy Mat. **5**, 1500646 (2015).

193. G. Tan, F. Shi, S. Hao, H. Chi, T. P. Bailey, L. D. Zhao, C. Uher, C. Wolverton, V. P. Dravid, and M. G. Kanatzidis, "*Valence Band Modification and High Thermoelectric Performance in SnTe Heavily Alloyed with MnTe*" J. Amer. Chem. Soc. **137**, 11507 (2015).

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4. C. Wolverton, G. Ceder, D. de Fontaine, and H. Dreyssé, "*An Ab-Initio Ground State Study with Fourth Nearest Neighbor Cluster Interactions for fcc Pd-V Alloys*", Phys. Rev. B (Rapid Communications) **45**, 13105 (1992).

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Prof. Christopher Wolverton – BOOK CHAPTERS

Y. Tang, C. Wolverton, and G. J. Snyder, "*Phase Diagram Study in n-CoSb3 Skutterudites*", in Materials Aspect of Thermoelectrics, ed. by C. Uher (CRC, Boca Raton), 2017.

Prof. Christopher Wolverton – PATENTS / INVENTION DISCLOSURES / DEFENSIVE PUBLICATIONS

Patents Granted:

9. J. Yang, D. Siegel, A. Sudik, A. Drews, S. Hirano, and C. Wolverton, "*Method of Enhancing Thermal Conductivity in Hydrogen Storage Systems* " (US8883117), 2014.

8. J. Yang, D. Siegel, A. Sudik, A. Drews, S. Hirano, and C. Wolverton, "*Method of Enhancing Thermal Conductivity in Hydrogen Storage Systems* " (US8418841), 2013.

7. J. Yang, A. Sudik, D. Siegel, S. Hirano, A. Drews and C. Wolverton, "*Hydrogen Storage Materials Containing Ammonia Borane*" (US8038980), 2011.

6. Syed A. Faheem, Gregory J. Lewis, J.W. Adriaan Sachtler, John J. Low, David A. Lesch, Paul M. Dosek, Christopher M. Wolverton, Donald J. Siegel, Andrea C. Sudik, Jun Yang, "*Multicomponent Hydrogen Storage Material*" US Patent (US7790133), 2010.

5. C. Wolverton, J. Low, and G. Lewis, "*High Density Hydrogen Storage Material*" US Patent (US7678362), 2010.

4. C. Wolverton, "*High Density Hydrogen Storage Material*" US Patent (US7625547), 2009.

3. A. Bogicevic, C. Wolverton, and D. Bauer, "A *miniaturized solid-oxide fuel cell*", European Patent (EP1300903), 2006.

2. "*Optimizing Heat Treatment of Aluminum Alloys by Predicting Thermal Growth*", C. Wolverton and J. Allison, US Patent (US6858103), 2005.

1. "*Ultrahigh Power Density Miniaturized Solid-oxide Fuel Cell*", A. Bogicevic, C. Wolverton, and D. Bauer, US Patent (US6495279), 2002.

Patents Pending/Defensive Publications:

9. C. Wolverton, S. Kirklin, S. Hao, D. H. Snydacker, V. Hegde, M. Aykol, S. Kim, Z. Lu, and Dane Morgan, "*Protective Cathode Coatings for Lithium Ion Batteries*", U. S. Patent Appl. 15/427,295 (Filed, Feb. 8, 2017).

8. C. Wolverton, D. Snydacker, V. Hegde, "*Protective Anode Coatings for High Energy Batteries*" International Patent Appl. PCT/US2017/021365 (Filed, Mar. 8, 2017) (provisional application No. 62/306,866 filed March 11, 2016).

7. C. Wolverton, D. Snydacker, V. Hegde, M. Aykol, "*Compounds for Lithium Extraction via Ion Exchange*", U.S. Patent Appl. 15/420,708 (Filed, Jan. 31, 2017)

6. J. Saal and C. Wolverton, "*Magnesium alloys having long-period stacking ordered phases*" (US2015086413-A1, 2015).

5. S. Kirklin and C. Wolverton, "*Transition metal silicides, stannides, and phosphides for use a negative electrodes in lithium secondary batteries*" (provisional application, 2012).

4. D. Siegel, C. Wolverton, V. Ozolins, A. Sudik, and J. Yang, "*Hydrogen Storage Materials*" (US Patent Application 20100233076, 2010).

3. A. Sudik, J. Yang, D. Siegel, and C. Wolverton, "*Methods of Enhancing Kinetic Properties of Hydrogen Storage Materials by Self-Catalysis*", (US Patent Application 20100068134, 2010).

2. A. Drews and C. Wolverton, "*Storage of Ammonia and Hazardous Chemicals in Polymer Microspheres*" (Defensive Publication, 2007).

1. "*A High Strength Cast Aluminum Alloy with Accelerated Response to Heat Treatment*", C. Wolverton, L. Godlewski, and J. Zindel (US Patent Application 20040213694, 2004).

Prof. Christopher Wolverton - INVITED TALKS

210. C. Wolverton, Yale University, Materials and Mechanical Eng. Colloquium, Oct. 2017.

209. C. Wolverton, Univ. Cambridge, Workshop - "From the Atom to the Material", Sept. 2017.

208. C. Wolverton, Materials Genome Workshop, Shanghai University, Shanghai, China, Sept. 2017.

207. C. Wolverton, Dupont Research Labs, Wilmington, DE, Aug. 2017.

206. C. Wolverton, NANOKorea, Seoul, Korea, July 2017.

205. C. Wolverton, National Institute of Materials Science, Materials Seminar, Tsukuba, Japan, July 2017.

204. C. Wolverton, Physics Next Workshop, Long Island, NY, May 2017.

203. C. Wolverton, PACRIM – 12th Pacific Rim Conference on Ceramics and Glass Technology, Hawaii, May 2017.

202. C. Wolverton, American Chemical Society Spring Meeting, San Francisco, Apr. 2017.

201. C. Wolverton, Distinguished Speaker Lecture Series, Univ. Alabama Huntsville, Mar. 2017.

200. C. Wolverton, APS March Meeting, New Orleans, Mar. 2017.

199. C. Wolverton, TMS Annual Meeting, San Diego, Feb. 2017.

198. C. Wolverton, International Conference on Computational Physics (ICCP10), Macau, China, Jan. 2017.

197. C. Wolverton, NREL Deep Decarbonization Workshop, Dec. 2016.

196. C. Wolverton, Department Colloquium, Case Western Reserve Univ., Dec. 2016.

195. C. Wolverton, "Computational Design of Nanostructured Thermoelectrics", MRS Fall Meeting, Boston, Dec. 2016.

194. C. Wolverton, "Computational Discovery of Novel Functional Heusler Compounds", MRS Fall Meeting, Boston, Dec. 2016.

193. C. Wolverton, Lorentz Center Workshop, "Open Databases Integration for Materials Design", Leiden, Netherlands, Oct. 2016.

192. C. Wolverton, IPAM Workshop, "Machine Learning meets Many Particle Problems", UCLA, Sept. 2016.

191. C. Wolverton, Vienna Young Researchers Workshop, Vienna, Sept. 2016.

190. C. Wolverton, CAMD Summer School, Copenhagen, Aug. 2016.

189. C. Wolverton, American Chemical Society Fall Meeting, Aug. 2016.

188. C. Wolverton, IU-MRS Meeting, Singapore, July 2016.

187. C. Wolverton, Next Generation Electrochemistry Summer School, UIC June 2016.

186. C. Wolverton, Electrochemical Society Annual Meeting, June 2016.

185. C. Wolverton, "Accelerating Materials Discovery with Data-Driven Computational Tools" NIST MGI Seminar Series, May 2016.

184. C. Wolverton, Department Colloquium, Univ. of Washington (Seattle), May 2016.

183. C. Wolverton, Department Colloquium, MIT, May 2016.

182. C. Wolverton, Department Colloquium, Johns Hopkins Univ., May 2016.

181. C. Wolverton, Department Colloquium, Washington Univ. at St. Louis, April 2016.

180. C. Wolverton, Invited Seminar, American Chemical Society, Mar. 2016.

179. C. Wolverton, German Physical Society, Mar. 2016.

178. C. Wolverton, "High-throughput Computational Search for Strengthening Precipitates in Alloys", TMS Annual Meeting, Feb. 2016.

177. C. Wolverton, "Assessing the Accuracy of DFT Formation Energies", TMS Annual Meeting, Feb. 2016.

176. C. Wolverton, Beijing Institute of Aeronautical Materials, Beijing, China, Dec. 2015.

175. C. Wolverton, MRS Fall Meeting, Boston, Nov. 2015.

174. C. Wolverton, UCSB Materials Colloquium, Nov. 2015.

173. C. Wolverton, Psi-K Meeting, San Sebastian, Spain, Sept. 2015.

172. C. Wolverton, ACS Fall Meeting, Boston, Aug. 2015.

171. C. Wolverton, New York Scientific Data Summit, New York, Aug. 2015.

170. C. Wolverton, FOMMS2015, Mt. Hood, Oregon, July 2015.

169. C. Wolverton, PTM2015, Whistler, Canada, July 2015.

168. C. Wolverton, CECAM Workshop, "Future Technologies in Automated Atomistic Simulations", Lausanne Switzerland, June 2015.

167. C. Wolverton, Workshop on Materials Science for Energy Storage, Trieste, Italy, May 2015.

166. C. Wolverton, MSE Colloquium, Univ. Illinois Urbana Champaign, May 2015.

165. C. Wolverton, Open Science Grid Workshop, Northwestern, Mar. 2015.

164. C. Wolverton, SRG Annual Meeting, Northwestern, Mar. 2015.

163. C. Wolverton, TMS Annual Meeting (Thermoelectrics), Orlando, FL, Mar. 2015.

162. C. Wolverton, TMS Annual Meeting (OQMD), Orlando, FL, Mar. 2015.

161. C. Wolverton, CECAM Workshop on Materials Discovery, Berlin, Germany, Feb. 2015.

160. C. Wolverton, MSE Colloquium, Cornell University, Nov. 2014.

159. C. Wolverton, LPSO2014, Kumamoto Japan, Oct. 2014.

158. C. Wolverton, General Motors Materials Seminar, Sept. 2014.

157. C. Wolverton, IU-MRS, Fukuoka, Japan, Aug. 2014.

156. C. Wolverton, 23rd International Union of Crystallography, Montreal, Canada, Aug. 2014.

155. C. Wolverton, Telluride Science and Technology Workshop, July 2014.

154. C. Wolverton, CIMTEC, 6th Forum on New Materials, Montecatini Terme, Italy, June 2014.

153. C. Wolverton, Workshop on Advanced Microscopy and Theoretical Calculations, Hamamatsu, Japan, May 2014.

152. C. Wolverton, Ford Motor Company, Dearborn, MI, Apr. 2014

151. C. Wolverton, TMS Annual Meeting (Thermoelectrics), San Diego, Feb. 2014

150. C. Wolverton, TMS Annual Meeting (Data Mining), San Diego, Feb. 2014

149. C. Wolverton, TMS Annual Meeting (Mg alloys), San Diego, Feb. 2014

148. C. Wolverton, NREL Materials Seminar, Nov. 2013

147. C. Wolverton, Institute of Pure and Applied Mathematics, UCLA, Nov. 2013

146. C. Wolverton, Dow Chemical Company, Midland, MI, Oct. 2013

145. Argonne National Laboratories, Materials Science Division Seminar, Aug. 2013.

144. 8th Pacific Rim International Congress on Advanced Materials and Processing (PRICM-8), Waikaloa, Hawaii, Aug. 2013.

143. Gordon Research Conference, "Hydrogen-Metal Systems", Barga, Italy, July 2013.

142. Plenary Lecture: 2nd World Congress on Integrated Computational Materials Engineering, Salt Lake City, July 2013.

141. Cambridge University, Materials Science Seminar, Cambridge, England, June 2013.

140. Thomas Young Centre, University College London, London, England, June 2013.

139. NSF Summer School "The Materials Genome: Current Practice and Future Promise" (3 lectures), June 2013.

138. Magnesium Workshop Madrid 2013: An International Workshop on Processing-Microstructure-Mechanical Property of Magnesium Alloys, Madrid, Spain, May 2013.

137. American Chemical Society, New Orleans, Apr. 2013.

136. University of Michigan, Materials Science Colloquium, Apr. 2013.

135. American Physical Society March Meeting, Baltimore, Mar. 2013.

134. German Physical Society, Regensburg, Mar. 2013.

133. TMS Annual Meeting, San Antonio (Thermoelectrics), Feb. 2013.

132. TMS Annual Meeting, San Antonio (High Throughput Data Mining), Feb. 2013.

131. MRS Fall Meeting, Boston, MA, Dec. 2012.

130. Drexel University, Materials Science Colloquium, Nov. 2012.

129. Univ. of California at Berkeley, Materials Science Colloquium, Oct. 2012.

128. International Symposium on Metal-Hydrogen Systems, Kyoto, Japan, Oct. 2012.

127. Workshop, “Harnessing the Materials Genome”, Vail, CO, Oct. 2012.

126. Jiao Tong University, Shanghai, China, Sept. 2012.

125. Beijing Institute of Aeronautical Materials, Beijing, China, Sept. 2012.

124. 15th International Workshop on Computational Electronics, Madison, WI, May 2012.

123. California Institute of Technology, Materials Science Colloquium, April 2012.

122. American Chemical Society Meeting, San Diego, Mar. 2012.

121. TMS Annual Meeting, Orlando, FL, Mar. 2012.

120. Yonsei University, Seoul, Korea, Feb. 2012.

119. Jiao Tong University, Shanghai, China, Aug. 2011.

118. Workshop, “Emerging Opportunities in Nanostructured Semiconductors”, June 2011.

117. CECAM Workshop, “Materials Infomatics”, May 2011.

116. IPAM Workshop, “Materials Design in Chemical Compound Space”, May 2011.

115. Materials Research Society Spring Meeting, San Francisco, April 2011.

114. American Chemical Society March Meeting, Anaheim, CA, Mar. 2011.

113. American Physical Society March Meeting, Dallas, TX, Mar. 2011.

112. TMS Annual Meeting, San Diego, CA, Feb. 2011.

111. Workshop, “Multiscale simulation of heterogeneous materials and coupling of thermodynamic models”, Leuven, Belgium, Jan. 2011.

110. Workshop, “Nano- and Surface Science Approaches to Production and Storage of Hydrogen", Noordwijkerhout, The Netherlands, Nov. 2010

109. CECAM Workshop, “Simulations and Experiments on Materials for Hydrogen Storage”, Dublin, Ireland Oct. 2010

108. Lawrence Livermore National Lab., July 2010

107. National Research Council, Committee on Condensed Matter Theory, April 2010

106. Northwestern University, Applied Math Colloquium, April 2010.

105. Materials Research Society Spring Meeting (Solar Thermochemical), San Francisco, April 2010.

104. Materials Research Society Fall Meeting (Energy Materials), Boston, November 2009.

103. Materials Research Society Fall Meeting (H2 Storage), Boston, November 2009.

102. TMS Materials Science and Technology Meeting, Pittsburgh, PA, Oct. 2009.

101. Indo-US Conference on Advanced Materials Research, Bangalore, India, Sept. 2009.

100. ACS Great Lakes Meeting, Lincolnshire, IL, May 2009.

99. Pacific Northwest National Laboratory, Richland WA, April 2009.

98. Materials Research Society Spring Meeting, San Francisco, April 2009.

97. Seminar – Denmark Technical University, Copenhagen, Apr. 2009.

96. American Physical Society March Meeting, Pittsburgh, PA, Mar. 2009.

95. TMS Annual Meeting, San Francisco, CA, Feb. 2009.

94. CompMat Workshop, Vienna, Austria, Jan. 2009.

93. Princeton University, Dept. Colloquium, Dec. 2008.

92. AsiaNano 2008 Conference, Singapore, Nov. 2008.

91. TMS Materials Science and Technology Meeting, Pittsburgh, PA, Oct. 2008.

90. Physics Department Colloquium, Brigham Young University, Provo Utah, Sept. 2008.

89. International Materials Research Congress, Cancun, Mexico, August 2008.

88. International Symposium on Metal Hydrogen Systems, Reykyavik, Iceland, June 2008.

87. Brookhaven National Lab., May 2008.

86. University of British Columbia (two colloquia given), April 2008.

85. Electrochemical Society Regional Chapter Meeting, Argonne National Lab., April 2008.

84. TMS Annual Meeting, Mar. 2008.

83. German Physical Society, Feb. 2008.

82. Workshop, "Measurement Needs for Local Structure Determination in Inorganic Materials" NIST, Washington DC, Feb. 2008.

81. Chemical Engineering Dept. Seminar, Univ. of Notre Dame, Nov. 2007.

80. Materials Science Dept. Colloquium, Michigan State Univ., Oct. 2007.

79. TMS Materials Science and Technology Meeting, Detroit, Sept. 2007 (H2 Storage).

78. TMS Materials Science and Technology Meeting, Detroit, Sept. 2007 (Al-Mg-Si Alloys).

77. 4th Conference of the Asian Consortium on Computational Materials Science, Seoul, Korea, Sept. 2007.

76. Chemistry Dept. Colloquium, Univ. of Nevada, Las Vegas, August 2007.

75. Seminar – General Motors Research Lab, August 2007.

74. Gordon Conference, "Metal-Hydrogen Systems", July 2007.

73. Conference, "Challenges in Multiscale Modeling of Materials", Stockholm, June 2007.

72. Workshop, “Theory meets Industry”, Vienna, June 2007.

71. Seminar - Argonne National Labs, March 2007.

70. TMS Annual Meeting, February 2007.

69. Seminar - Sandia National Labs, Albequerque, February 2007.

68. International Conference on Aluminum Alloys 10, Vancouver, July 2006.

67. Computational Science Workshop (CSW2006), Tsukuba, Japan, April 2006.

66. American Physical Society Meeting, March 2006.

65. TMS Annual Meeting, March 2006.

64. Workshop , “Ab-initio description of iron and steel”, Ringberg Castle, Germany, February, 2006.

63. Seminar - Pacific Northwest National Labs, January, 2006.

62. Seminar – CEA, Saclay, France, December, 2005.

61. Workshop – “Rational Design of Catalysts and Sorbents”, Institut de Francais du Petrole (IFP), Lyon, France, December 2005.

60. Materials Science Colloquium, MIT, October, 2005

59. Materials Science Colloquium, Cornell University, September, 2005

58. Psi-k Electronic Structure Conference, September, 2005.

57. Seminar – KTH, Stockholm, Sweden, September, 2005.

56. SINTEF/Univ. Trondheim, Norway, June, 2005.

55. Lecture in MIT/Singapore/Univ. Cambridge Course - “Atomistic Computer Modeling of Materials”, April 2005.

54. TMS 2005 Annual Meeting, San Francisco, February, 2005.

53. Invited Panel Member - Institute for Mathematics and its Applications Workshop, Univ. of Minnesota, Nov. 2004

52. Institute for Energy Technology, Oslo, Norway, September, 2004

51. European Materials Research Society Meeting, Warsaw, Poland, September, 2004

50. Materials Design Workshop, Seattle, June 2004.

49. Lecture in MIT/Singapore/Univ. Cambridge Course - “Atomistic Computer Modeling of Materials”, April 2004.

48. Aerospace Engineering and Mechanics Department Seminar, Univ. of Minnesota, Minneapolis, April 2004

47. Materials Science Department Seminar, Univ. of Michigan, November 2003

46. Physics Colloquium, California State Univ., Northridge, May 2003

45. John Dorn Memorial Lecture, Northwestern University, May 2003

44. Lecture in MIT/Singapore/Univ. Cambridge Course - “Atomistic Computer Modeling of Materials”, April 2003

43. TMS Annual Meeting, San Diego, March 2003

42. Physics Dept. Seminar, Michigan State Univ., Nov. 2002

41. Institute for Pure and Applied Mathematics Workshop: “Modeling and Simulation for Materials”, UCLA, Nov. 2002

40. NSF Workshop, “Opportunities in Materials Theory”, Washington DC, October 2002

39. Lecture in MIT/Singapore Course - “Atomistic Computer Modeling of Materials”, May 2002

38. TMS Annual Meeting, Seattle, February 2002.

37. Seminar, Institute for Advanced Materials, Brno, Czech Republic, January 2002

36. Physics Colloquium, Univ. of Erlangen, Germany, January 2002

35. Max-Planck Institute Workshop on Alloy Theory, Ringburg Castle, Germany, January 2002

34. ACerS Advanced Ceramics Meeting (SOFC), Cocoa Beach, January 2002

33. TMS Fall Meeting (CALPHAD session), Indianapolis, November 2001

32. TMS Fall Meeting (Alloy Design session), Indianapolis, November 2001

31. Condensed Matter Seminar, Ohio State University, October 2001

30. International Workshop on the Thermodynamic and Structural Properties of Materials, Avignon, France, September 2001

29. Condensed Matter Seminar, Chalmers University, Göttinberg, Sweden, September 2001

28. Computational Materials Science Seminar Series, Oak Ridge National Laboratory, August 2001

27. Materials Science Seminar, Carnegie Mellon Univ., April 2001

26. Invited Seminar, Alcoa Technical Center, April 2001

25. Computational Materials Science Network, Santa Fe, January 2001

24. Materials Science Department Colloquium, Penn State University, November 2000

23. Chemistry Department Colloquium, Univ. of Pennsylvania, Fall 2000

22. American Ceramic Society Meeting, St. Louis, April 2000

21. American Physical Society (APS) 2000 Meeting, Minneapolis, March 2000

20. Materials Research Society (MRS) Fall Meeting, December 1999

19. Electrochemical Society Meeting, Honolulu, October 1999

18. Physics Department Colloquium, Central Michigan University, September 1999

17. International Workshop on "Thermodynamics and Structural Properties of Alloy Materials", Aruba, June 1999

16. Workshop on New Methods in Electronic Structure, Univ. of Illinois, Urbana-Champaign, May 1999

15. Invited Seminar, Ford Motor Research Laboratories, October 1998

14. Physics Departmental Colloquium, Colorado School of Mines, September 1998

13. Physics Departmental Colloquium, University of Houston, February 1998

12. TMS Spring Meeting, Hume-Rothery Symposium, February 1998

11. Materials Research Society (MRS) Fall Meeting, December 1997

10. MSU Workshop, “Local Structure from Diffraction”, August 1997

9. NSF/CNRS Workshop on Alloy Theory, Mt. St. Odile Monastery, France. October 1996

8. CECAM Workshop, “Theoretical Predictions of Alloy Phase Stability”, Lyon, France. June 1996

7. Materials Research Society (MRS) Spring Meeting, April 1996

6. The Minerals, Metals, and Materials Society (TMS), 1995 Materials Week, October 1995

5. Departmental Colloquium, Colorado School of Mines, September 1994

4. Computational Methods for the Structure of Alloys, Univ. of Kentucky, June 1993

3. Invited Seminar, Massachusetts Institute of Technology, November 1992

2. Computational Methods for the Structure of Alloys, Univ. of Kentucky, June 1992

1. Computational Methods for the Structure of Alloys, Univ. of Kentucky, June 1991

Prof. Christopher Wolverton – NON-REFEREED PUBLICATIONS

27. V. Ozolins, A. R. Akbarzadeh, H. Gunaydin, K. Michel, C. Wolverton, and E. Majzoub, “First-principles computational discovery of materials for hydrogen storage”, SCIDAC 2009: Scientific Discovery Through Advanced Computing, Journal of Physics Conference Series, Volume 180 (2009).

26. M. Veenstra, A. Sudik, J. Yang, and C. Wolverton, "*On-Board Hydrogen Storage: Bridging the Gap from the Hydrogen Lab to the Hydrogen Vehicle*", NHA Hydrogen Conference 2006.

25. A. Sudik, M. Veenstra, and C. Wolverton, "*Potential of Ammonia and Ammonia-Related Carriers in a Hydrogen Economy*", Ford Tech. Report, (2006).

24. V. Vaithyanathan, C. Wolverton, and L. Q. Chen, *"Modeling Precipitate Microstructure Evolution in Alloys With First-Principles Energetic Information",* Materials Science Forum 449, **19** (2004).

23. C. Ravi and C. Wolverton, *"Critical Assessment of Thermodynamic Databases for 3xx and 6xxx Automotive Aluminum Alloys",* Ford Technical Report, SRR-2004-0080.

22. L. Q. Chen, S. Hu, V. Vaithyanathan, C. Jiang, J. Wang, Z.-K. Liu, C. Wolverton, J. Murray, H. Weiland, and S. Müller, *"Computer Modeling of Phase Transformations in Al Alloys"* in *Metallurgical Modeling for Aluminum Alloys*, ASM International, Materials Park, OH, ed. M. Tiryakioglu and L. Lalli, p. 133 (2003).

21. M. Li, R. Vijayaraghavan, C. Wolverton, and J. E. Allison, "*Simulation of Local Microstructures and Thermal Growth of a Cast 319 Aluminum Alloy Component*", in *Metallurgical Modeling for Aluminum Alloys*, ASM International, Materials Park, OH, ed. M. Tiryakioglu and L. Lalli, p. 79 (2003).

20. C. Wolverton, L. G. Godlewski, and J. Zindel, "*Accelerating the heat treatment response of a 319-type Al alloy: Microalloying with Sn*", Ford Research Laboratory Technical Report SRR-2001-0249 (2001).

19. C. Wolverton and J. E. Allison, "*Thermal growth during heat treatment of Al 319: A predictive model*", Ford Research Laboratory Technical Report SRR-2001-0168 (2001).

18. J. E. Allison, R. Vijayaraghavan, and C. Wolverton, "*Virtual Aluminum Castings*", Ford Research Laboratory Research Highlight **9**, 2 (2001).

17. W. F. Schneider, K. C. Hass, M. L. Greenfield, C. Wolverton, A. Bogicevic, D. J. Mann, and E. B. Stechel, "*Chemical and Materials Simulation at Ford Motor Company*", in Foundations of Molecular Modeling and Simulation, P. T. Cummings, P. R. Westmoreland, and B. Carnahan, eds. AIChE Symposium Series No. 325, **97**, 19 (2001).

16. C. Wolverton, "*First-Principles Theory of Coherent Precipitation in Al Alloys*", Proceedings of the International Conference on Intergranular and Interface Boundaries", Prague, Czech Republic, Trans Tech Publications, p. 469 (1999).

15. C. Wolverton and A. Zunger, "*First-Principles Theory of Cation and Vacancy Ordering in Li_xCoO_2*", Mat. Sci. Res. Proc. **496**, 77 (1998).

14. D. de Fontaine, M. Asta, R. McCormack, and C. Wolverton, "*First-Principles Thermodynamics of Alloys*", in New Horizons for Materials, edited by P. Vincenzini, (TECHNA, Faenza, Italy, 1995), p. 241-246.

13. C. Wolverton and D. de Fontaine, "*Site Substitution of Ternary Additions to Ni_3Al (γ') from Electronic Structure Calculations*," in Alloy Modeling and Design, G. M. Stocks and P. E. A. Turchi, Eds. (TMS, 1993).

12. R. McCormack, G. Ceder, C. Wolverton, and D. de Fontaine, "*First-Principles Ternary Phase Equilibria*," in Alloy Modeling and Design, G. M. Stocks and P. E. A. Turchi, Eds. (TMS, 1993).

11. D. de Fontaine, A. Finel, H. Dreyssé, M. Asta, R. McCormack, and C. Wolverton, in Metallic Alloys, NATO ASI Series, **256**, 1994, p. 205.

10. G. Ceder, P. D. Tepesch, C. Wolverton, and D. de Fontaine, "*Ab-initio Computation of the Pd-V Phase Diagram*," in Statics and Dynamics of Alloy Phase Transformations, edited by P. E. A. Turchi and A. Gonis, NATO ASI Series (Plenum Pres, New York, 1994).

9. P. D. Tepesch, G. Ceder, C. Wolverton, and D. de Fontaine, "*An ab-initio Calculation of the Pd-V fcc Superstructure Phase Diagram with Fourth Nearest Neighbor Cluster Interactions*," Mat. Res. Soc. Proc., p. 129 (1993).

8. C. Wolverton and D. de Fontaine, "*Electronic Structure of Ordered and Disordered Ternary Intermetallics*," Mat. Res. Soc. Proc. p. 431 (1993).

7. C. Wolverton, D. de Fontaine, H. Dreyssé, and G. Ceder, "*Electronic Structure of Substitutionally Disordered Alloys: Direct Configurational Averaging*," Mat. Res. Soc. Proc. **278**, 307 (1992).

6. C. Wolverton, G. Ceder, D. de Fontaine, and H. Dreyssé, "*Ground State Searches in fcc Intermetallics*," Mat. Res. Soc. Proc. **253**, 243 (1992).

5. D. de Fontaine, C. Wolverton, G. Ceder, and H. Dreyssé, "*Cluster Expansion of fcc Pd-V Intermetallics*," in C. T. Liu et al. (eds.), Ordered Intermetallics - Physical Metallurgy and Mechanical Behavior, NATO ASI Series E: Applied Sciences 213, 61 (1992).

4. D. de Fontaine, M. Asta, C. Wolverton, and H. Dreyssé, "*First-Principles Calculations of Phase Diagrams*," Proc. Of JIMIS-6, Sendai, Japan, pp. 199-207 (1991).

3. H. Dreyssé, L. T. Wille, G. Ceder, C. Wolverton, and D. de Fontaine, "*The Electronic Structure of Disordered Alloys with or without Surface*," Proc. of 20th Annual International Symposium on Electronic Structure of Solids, Gaussig, 1990 (Nova Science Pub., New York, 1991).

2. D. de Fontaine, M. Asta, C. Wolverton, and H. Dreyssé, "*CVM Approach to Alloy Theory*," Joint Research Report, Monbusho International Scientific Research Program sponsored by the Japanese Ministry of Education, Science, and Culture, (1990).

1. C. Wolverton, H. Dreyssé, and D. de Fontaine, "*A Comparison of the Direct Configurational Averaging and Connolly-Williams Methods of Obtaining Effective Pair Interactions in Substitutionally Disordered Alloys*," Mat. Res. Soc. Proc., (1990).