Curriculum Vitae

Qi-Jun Hong

Assistant Professor
Arizona State University

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Education

Ph.D., Physical Chemistry, California Institute of Technology, October 2014.
Thesis title: Methods for melting point calculation
Advisor: Prof. Axel van de Walle
Thesis Committee: Profs. William A. Goddard, III (Chair), Thomas F. Miller, Nathan S. Lewis
GPA: 4.1/4.3

B.S., Chemistry, Fudan University, 2009.
Advisor: Prof. Zhi-Pan Liu
GPA: 3.86/4.0 (2/101)

Professional Experience

Assistant Professor — August 2021−Present
Materials Science and Engineering
School for Engineering of Matter, Transport and Energy
Arizona State University

Applied Scientist II — November 2020−August 2021
Machine Learning
Amazon.com Inc.

Senior Research Scientist — November 2014−November 2020
Materials Science and Engineering
School of Engineering
Brown University (under the supervision of Axel van de Walle)

Professional Activities

Developer of the *Solid and Liquid in Ultra Small Coexistence with Hovering Interfaces (SLUSCHI)* code, a software package available at https://faculty.engineering.asu.edu/hong/ that enables first principles calculations of melting temperature, heat of fusion, enthalpy, *etc. SLUSCHI* has been downloaded more than 3,000 times with its website visited 15,000 times worldwide.

Developer of the *Materials Properties Predicction (MAPP)* project, a framework and cyber infrastructure available at the website https://faculty.engineering.asu.edu/hong/ that enables rapid calculations of melting temperature, heat of fusion, enthalpy, *etc. MAPP* has been utilized by users across the world by more than 7,000 (web) and 300,000 (API) times.

Referee for *Nature*, *Physical Review Letters*, *Physical Review B*, *Physical Review E*, *Chemical Engineering Journal*, *Scientific Reports*, *Acta Materialia*, *Journal of Chemical Theory and Computation*, *Journal of Applied Physics*, *CALPHAD*, *Journal of Alloys and Compounds*, and *Computational Materials Science*.

Grants

1. Co-PI, Collaborative Research: Rare Earth Materials Under Extreme Conditions, National Science Foundation, $636,980 (Hong's share: $255,000), Collaborators: Alex Navrotsky (ASU), Axel van de Walle (Brown), June 2022 - June 2026.
2. Co-PI, DOD ARO MURI: Emergent Refractory Behaviors in Earth and Extraterrestrial Materials, Army Research Office, Department of Defense, $6,000,000 (Hong's share: $500,000) Collaborators: Alex Navrotsky, Hongwu Xu (ASU), Beth Opila, Bi-Cheng Zhou, Patrick Hopkins (University of Virginia), August 2023 - August 2028.
3. Co-PI, DOE Earthshots: Fundamental Studies of Hydrogen Arc Plasmas for High-efficiency and Carbon-free Steelmaking, Department of Energy, $6,000,000 (Hong's share: $536,667) Collaborators: Sridhar Seetharaman, Christopher Muhich, Kumar Ankit (ASU), University of Texas at Austin, National Renewable Energy Laboratory (NREL), October 2023 - October 2026.
4. Inaugural awardee, the Navrotsky Early Career Award, $50,000, July 2023 - July 2026.
5. PI, grant for XSEDE/ACCESS supercomputer time allocation (2021, yearly).

Current Group Members

1. Ligen Wang (Research scientist)
2. Audrey CampBell (PhD student)
3. Si-Da Xue (PhD student)
4. Dallin Fisher (PhD student)
5. John Grimm (MS student)
6. Philip Wurzner (Visiting student from TU Delft)

Alumni

1. Ahmad Alqaisi (MS student)
2. Aanand Mehta (High school student)

Course Taught at ASU

1. MSE 457/598: Quantum Mechanics: Atoms and Solids. 2023 Fall Student Evaluation: 4.74/5.
2. MSE 458/515: Electronic, Magnetic, and Optical Properties
3. MSE 415: Computational and Numerical Methods (scheduled Fall 2024)

Service at ASU

1. SCENE Program Mentor. The SCience and ENgineering Experience (SCENE) provides cutting-edge science research experience to high school sophomores, juniors and seniors.
2. Machine learning faculty search committee, 2022-2023

Publications

Citations: 1480 h-index: 18 (March 2024)

42. **Q.-J. Hong**, S. V. Ushakov, Ligen Wang, A. Navrotsky, and A. van de Walle, Cubic to hexagonal phase transition of Er_2O_3, Ho_2O_3 and Tm_2O_3. In preparation.

41. Ligen Wang and **Q.-J. Hong**, High temperature crystal structure prediction via density functional theory. In preparation.

40. A. CampBell, Ligen Wang, S.-H. Shim, and **Q.-J. Hong**, Iron melting curve from ab initio molecular dynamics calculations. In preparation.

39. A. M. Alqaisi, H. Zhuang, and **Q.-J. Hong**, A computational study on melting point of Si-Ge-Sn high entropy alloy. In preparation.

38. A. CampBell and **Q.-J. Hong**, The integration of VASP 6's Machine learning algorithms into the Solid and Liquid in Ultra Small Coexistence with Hovering Interfaces code to for melting point determination. In preparation.

37. **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. Submitted.

36. S.-D. Xue and **Q.-J. Hong**, Materials Properties Prediction (MAPP): Empowering the prediction of material properties solely based on chemical formulas, *arXiv*, 2023.

35. **Q.-J. Hong**, Deep learning for CALPHAD modeling: Universal parameter learning solely based on chemical formula, *arXiv*, 2023, arXiv:2307.04283.

34. Aanand Mehta and **Q.-J. Hong**, QJHong Model for Novel Coronavirus Disease 2019 (COVID-19) in the United States, *medRxiv*, 2023, https://doi.org/10.1101/2023.07.30.23293233.

33. X. Hu, Z. Zhao, Y. Zhao, X. Wang, S. Sainio, D. Nordlund, C. Ruse, X.-D. Zhou, S. Boettcher, D. Hou, **Q.-J. Hong**, L. Mu, Interfacial degradation of the NMC/Li6PS5Cl composite cathode in all-solid-state batteries, *Journal of Materials Chemistry A*, In Press.

32. B. Brugman, Y. Han, L. Leinbach, K. Leinenweber, A. van de Walle, S. Ushakov, **Q.-J. Hong**, and A. Navrotsky, Computationally led high pressure synthesis and experimental thermodynamics of rocksalt yttrium monoxide, *Chemistry of Materials*, 36:332, 2024.

31. S. Hao, **Q.-J. Hong**, and M. C. Gao, A prediction of the thermodynamic, thermophysical, and mechanical properties of $CrTaO_4$ from first principles, *Journal of the American Ceramic Society*, 106:7654, 2023.

30. S. V. Ushakov, **Q.-J. Hong**, D. Gilbert, A. van de Walle, and A. Navrotsky, Thorium and rare earth compounds with rocksalt structures, *Materials*, 16:1350, 2023.

29. **Q.-J. Hong**, S. V. Ushakov, K. Lilova, A. Navrotsky, and S.J. McCormack, Structure and thermodynamics of oxides/carbides/nitrides/borides at high temperature (STOHT2). *ACerS Bulletin*, 102:28, 2023.

28. **Q.-J. Hong**, A. van de Walle, S.V. Ushakov, and A. Navrotsky, Integrating computational and experimental thermodynamics of refractory materials at high temperature, *CALPHAD*, 79:102500, 2022. (Invited)

27. **Q.-J. Hong**, S.V. Ushakov, A. Navrotsky, and A. van de Walle, Melting temperature prediction using a graph neural network model: from ancient minerals to new materials, *PNAS - Proceedings of the National Academy of Sciences*, 119:e2209630119, 2022.

26. **Q.-J. Hong**, Melting temperature prediction via first principles and deep learning, *Computational Materials Science*, 214:111684, 2022. (Invited)

25. E. Y. Cramer, et al., The United States COVID-19 Forecast Hub dataset, *Scientific Data*, 9:1, 2022.

24. E. Y. Cramer, et al., Evaluation of individual and ensemble probabilistic forecasts of COVID-19 mortality in the US, *PNAS - Proceedings of the National Academy of Sciences*, 119:e2113561119, 2022.

23. **Q.-J. Hong**, A melting temperature database and a neural network model for melting temperature prediction, *arXiv*, arXiv:2110.10748v2, 2021.

22. H. Chen, **Q.-J. Hong**, S.V. Ushakov, A. Navrotsky, and A. van de Walle, A simple method for computing the formation energies of metal oxides. *Computational Materials Science*, 198:110692, 2021.

21. **Q.-J. Hong**, J. Schroers, D. Hofmann, S. Curtarolo, M. Asta, and A. van de Walle, Theoretical prediction of high melting temperature for a Mo-Ru-Ta-W HCP multi-principal element alloy, *npj Computational Materials*, 7:1, 2021.

20. **Q.-J. Hong** and A. van de Walle, Re-entrant melting of sodium, magnesium and aluminum, and its general trend, *Physical Review B Rapid Communications*, 100:140102, 2019.

19. S. V. Ushakov, A. Navrotsky, **Q.-J. Hong**, and A. van de Walle, and, Carbies and nitrides of Zirconium and Hafnium, *Materials*, 12:2728, 2019.

18. A. van de Walle and **Q.-J. Hong**, Assessing phase diagram accuracy, *Journal of Phase Equilibria and Diffusion*, 2:170, 2019.

17. M. Fyhrie, **Q.-J. Hong**, D. Kapush, S. V. Ushakov, A. van de Walle, and A. Navrotsky, Fusion enthalpies of Tm_2O_3, Yb_2O_3, and Lu_2O_3 from drop and catch calorimetry and first principles calculations, *Journal of Chemical Thermodynamics*, 132:405, 2019.

16. **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_2 and HfO_2, *Scientific Reports*, 8:14962, 2018.

15. **Q.-J. Hong** and A. van de Walle, A tetrahedron tiling method for crystal structure prediction, *Physical Review Materials Rapid Communications*, 1:020801, 2017.

14. A. van de Walle, R. Sun, **Q.-J. Hong**, S. Kadkhodaei, Software tools for high-throughput CALPHAD from first-principles data, *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, 58:70, 2017.

13. A. van de Walle, S. Kadkhodaei, R. Sun, **Q.-J. Hong**, Epicycle method for elasticity limit calculations, *Physical Review B*, 95:144113, 2017.

12. 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 calculation, *Acta Materialia*, 124:204, 2017.

11. S. Kadkhodaei, **Q.-J. Hong** and A. van de Walle, Free energy calculation of mechanically unstable but dynamically stabilized bcc titanium, *Physical Review B*, 95:064101, 2017.

10. **Q.-J. Hong** and A. van de Walle, A user guide for SLUSCHI (Solid and Liquid in Ultra Small Coexistence with Hovering Interfaces). *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, 52:88, 2016. (Invited article)

9. 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: Computer Coupling of Phase Diagrams and Thermochemistry*, 51:133, 2015.

8. **Q.-J. Hong** and A. van de Walle. Prediction of the material with highest known melting point from *ab initio* molecular dynamics calculations. *Physical Review B Rapid Communications*, 92:020104(R), 2015. (Featured in the Washington Post, in Materials Today, in IEEE spectrum, in the Tech insider, in the Daily Mail (UK), on the Brown news site and in the Brown Engineering Magazine, among other media outlets.)

7. A. van de Walle, **Q.-J. Hong**, S. Kadkhodaei and R. Sun, The free energy of mechanically unstable phases. *Nature Communications*, 6:7559, 2015.

6. **Q.-J. Hong**, S. V. Ushakov, A. Navrotsky and A. van de Walle, Combined computational and experimental investigation of the refractory properties of $La_2Zr_2O_7$. *Acta Materialia*, 84:275, 2015.

5. A. van de Walle, **Q.-J. Hong**, L. Miljacic, C. Balaji Gopal, S. Demers, G. Pomrehn, A. Kowalski and P. Tiwary. *Ab initio* calculation of anisotropic interfacial excess free energies. *Physical Review B*, 89:184101, 2014.

4. **Q.-J. Hong** and A. van de Walle. Solid-liquid coexistence in small systems: A statistical method to calculate melting temperatures. *Journal of Chemical Physics*, 139:094114, 2013.

3. **Q.-J. Hong** and A. van de Walle. Direct first-principles chemical potential calculations of liquids. *Journal of Chemical Physics*, 137:094114, 2012.

2. **Q.-J. Hong** and Z.-P. Liu. Mechanism of CO_2 hydrogenation over $Cu/ZrO_2(\bar{2}12)$ interface from first-principles kinetics Monte Carlo simulations. *Surface Science*, 604:1869, 2010.

1. Q.-L. Tang, **Q.-J. Hong**, and Z.-P. Liu. CO_2 fixation into methanol at Cu/ZrO_2 interface from first principles kinetic Monte Carlo. *Journal of Catalysis*, 263:114, 2009.

Talks

34. The integration of VASP 6's machine learning algorithms into the Solid and Liquid in Ultra Small Coexistence with Hovering Interfaces code to for melting point determination
Audrey CampBell and Qi-Jun Hong. TMS annual meeting, Orlando, FL (2024) (Scheduled talk by student)

33. Deep Learning for Large-scale Prediction of Melting Temperature and Materials Properties
Qi-Jun Hong. SIPS: Navrotsky International Symposium 2023, Panama (2023). (Invited talk)

32. Deep Learning for Large-scale Prediction of Melting Temperature and Materials Properties
Qi-Jun Hong. Zhejiang University, China, Virtual (2023). (Invited talk)

31. Deep Learning for Large-scale Prediction of Melting Temperature and Materials Properties
Qi-Jun Hong. Materials Science and Technology annual meeting, Columbus, OH (2023). (Invited talk)

30. Deep Learning and DFT for Prediction of Melting Temperature and Materials Properties
Qi-Jun Hong. MURI Kick-off Meeting, Charlottesville, VA (2023). (Invited talk)

29. Deep Learning for Large-Scale Prediction of Melting Temperature and Materials Properties
Qi-Jun Hong. Calphad XL, Cambridge, MA (2023).

28. Melting temperature prediction via integrated first principles and deep learning
Qi-Jun Hong. TMS annual meeting, San Diego, CA (2023). (Invited talk)

27. Computation for high temperature and high pressure materials properties
Qi-Jun Hong. MOTU External Advisory Meeting, Tempe, AZ (2023). (Invited talk)

26. Mapping chemical formula to materials properties: The MAterials Properties Prediction (MAPP) Project
Qi-Jun Hong. MOTU Lunch Talk, Tempe, AZ (2022). (Invited talk)

25. Design and discovery of high-melting-point materials from first principles and deep learning.
Qi-Jun Hong. STOHT2 Conference, Tempe, AZ (2022).

24. Design of high melting point materials via deep learning and first principles.
Qi-Jun Hong. Materials Science and Technology annual meeting, Pittsburg, PA (2022).

23. Design and discovery of high-melting-point materials from ab initio and deep learning.
Qi-Jun Hong. Iowa State University, Virtual (2022). (Invited talk)

22. Melting temperature prediction via first principle and deep learning.
Qi-Jun Hong. MOTU Celebration, Tempe, AZ (2022). (Invited talk)

21. Melting temperature prediction via first principle and deep learning.
Qi-Jun Hong. Navrotsky Group Talk, Tempe, AZ (2022). (Invited talk)

20. Design of high-melting-temperature materials via first principles and deep learning.
Qi-Jun Hong. Telluride Workshop, Telluride, CO (2022). (Invited talk)

19. Design of high-melting-point materials via first principles and deep learning.
Qi-Jun Hong. Calphad XLIX, Stockholm, Sweden (2022).

18. Materials design of high-melting-point materials from first principles, database, and machine learning.
Qi-Jun Hong. TMS annual meeting, Anaheim, CA (2022). (Invited talk)

17. Materials design and discovery of high-melting-point and high-pressure materials from first principles and deep learning.
Qi-Jun Hong. ASU Chem 501, Tempe, AZ (2022). (Invited talk)

16. Materials design and discovery of high-melting-point materials from first principles and deep learning.
Qi-Jun Hong. University of Colorado at Colorado Springs, Colorado Spring, CO (2022). (Invited talk)

15. Materials design and discovery of high-melting-point materials.
Qi-Jun Hong. University of Science and Technology of China, Virtual (2021). (Invited talk)

14. Experimental and computational thermodynamics of refractory materials at high temperature.
Alexandra Navrotsky, Axel Van de Walle, Sergey Ushakov and Qi-Jun Hong. Calphad Global, Virtual (2021). (Plenary talk)

13. Ab initio computational discovery of high melting temperature materials.
Qi-Jun Hong. Arizona State University (2021). (Invited talk)

12. Reentrant melting of sodium, magnesium and aluminum and possible universal trend.
Qi-Jun Hong and Axel van de Walle. Calphad XLVII, Querétaro, México (2018).

11. Reentrant melting of sodium, magnesium and aluminum and possible universal trend.
Qi-Jun Hong and Axel van de Walle. TMS annual meeting, Phoenix, AZ (2018).

10. Software tools for high-throughput CALPHAD from first-principles data.
Axel van de Walle, Ruoshi Sun, Qi-Jun Hong, Sara Kadkhodaei. TMS annual meeting, Phoenix, AZ (2018). (Invited talk)

9. A tetrahedron tiling method for crystal structure prediction.
Qi-Jun Hong and Axel van de Walle. TMS annual meeting (2017).

8. Calculations of heat of fusion and melting temperature via an automated ab initio tool.
Qi-Jun Hong and Axel van de Walle. STOHT16 (International Research Conference on Structure and Thermodynamics of Oxides at High Temperature), UC Davis, Davis CA (2016) (Poster).

7. Prediction of the material with highest know melting point via an automated ab initio melting point calculation tool.
Qi-Jun Hong and Axel van de Walle. Materials Science and Technology meeting, Columbus, OH (2015).

6. Ab initio prediction of the material with highest known melting point.
Qi-Jun Hong and Axel van de Walle. TMS annual meeting (2015).

5. Prediction of the material with highest know melting point via an automated ab initio melting point calculation tool.
Qi-Jun Hong and Axel van de Walle. University of Wisconsin, Madison, WI (2015) (Poster).

4. Ab initio prediction of the material with highest known melting point.
Qi-Jun Hong and Axel van de Walle. MRS fall meeting (2014).

3. Solid-liquid coexistence in small systems: a statistical method to calculate melting temperatures.
Qi-Jun Hong and Axel van de Walle. NIST, Gaithersburg, MD (2014).

2. Solid-liquid coexistence in small systems: a statistical method to calculate melting temperatures.
Qi-Jun Hong and Axel van de Walle. TMS annual meeting, San Diego, CA (2014).

1. Direct first-principles chemical potential calculations of liquids.
Qi-Jun Hong and Axel van de Walle. MRS fall meeting, Boston, MA (2012).

Prizes, Awards and press coverage

2024	CALPHAD Young Leader Award.
2023	Professor of Impact, nominated and awarded by students in MSE458/515.
2023	DOE Earthshots funding team was featured in ASU news and Full Circle Journal of Fulton School of Engineering.
2023	Inaugural Navrotsky Early Career Award. Qi-Jun Hong was featured in ASU news and Full Circle Journal of Fulton School of Engineering.
2022	MOTU Celebration talk "Melting temperature prediction via first principle and deep learning" was featured in ASU news.
2022	Paper "Melting temperature prediction using a graph neural network model: from ancient minerals to new materials" was featured in Full Circle Journal of Fulton School of Engineering, phys.org, among other news outlets.
2021	Finalist for Rising Star in Computational Materials Science 2021, Elsevier.
2020	QJHong COVID19 model predictions were featured by Boston 25 News three times from October to December.
2019	Paper "Re-entrant melting of sodium, magnesium and aluminum: General trend" was featured on "News from Brown".
2015	Paper "Prediction of the material with highest known melting point from *ab initio* molecular dynamics calculations" was featured in the Washington Post, *Materials Today*, the *Daily Mail*, *IEEE Spectrum*, *Science*, among other popular journals.
2006, 2007	1st prize, People's Scholarship in Fudan University
2006	Excellent student in Fudan University
2005	1st prize, Scholarship for Excellent Freshman in Fudan University
2005	Gold medal in National Chemistry Olympiad • Ranked 17th in all the 150,000 participants in P. R. China • Awarded by Chinese Chemical Society
2004	1st prize in National Chemistry Olympiad (Shanghai), ranked 2nd.