Aidan P. Thompson

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EDUCATION

Ph.D., Chemical Engineering, University of Pennsylvania, 1994

M.S.E, Chemical Engineering, University of Pennsylvania, 1991

B.S., Chemical Engineering, University College Dublin, National University of Ireland, 1986

EMPLOYMENT HISTORY

Distinguished Member of the Technical Staff
Sandia National Laboratories (May 2021- Present)

Principal Member of the Technical Staff
Sandia National Laboratories (Oct. 2005 - May 2021)

Senior Member of the Technical Staff
Sandia National Laboratories (Mar. 1999 - Oct. 2005)

Limited Term Employee
Sandia National Laboratories (Jul. 1997 - Mar. 1999)

Senior Research Scientist
Union Camp Corporation (Sept. 1994 - Jun. 1997)

RESEARCH INTERESTS

Data-Driven Interatomic Potentials: spectral neighbor analysis potential (SNAP); automated training and validation software (FitSNAP); rotation-invariant atomic environment descriptors; ab initio training data generation

Atomistic Materials Simulation: LAMMPS software development; interatomic potential development; equilibrium and non-equilibrium molecular dynamics; kinetic Monte Carlo; equilibrium Monte Carlo; statistical physics

High-Performance Computing: scalable parallel algorithms; code optimization for advanced architectures; software development for leadership computing platforms

PROFESSIONAL RECOGNITION AND AWARDS

8. Siva Rajamanickam, Attila Cangi, Lenz Fiedler, Normand Modine, Aidan Thompson, Jon Vogel, and Adam Stephens. R&D 100 Award for MALA Materials Learning Algorithm. R&D 100 Award Competition and Expo, Coronado, California, 2023.

7. Aidan Thompson. Fellow of the American Physical Society, Division of Computational Physics (DCOMP). 2023.

6. Aidan Thompson. Plenary Talk: Molecular Dynamics Simulation: Engine of Discovery or Bridge to Nowhere? 21st Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter, Portland, 2019.

5. Steve Plimpton and Aidan Thompson. R&D 100 Award for LAMMPS. R&D 100 Award Competition and Expo, November, Orlando, 2019.

4. Aidan Thompson. Individual Performance Award. Presented by Laboratory Director Steve Rottler, "In recognition for developing models to simulate detonation of energetic materials", 2015.

3. Aidan Thompson. Individual Performance Award. Presented by 1400 Director Bill Camp for Demonstration of GRASP Performance on CPlant, 2004.

2. Aidan Thompson and Marcus Martin. First Place Prize: Viscosity of n-nonane/isopropanol mixtures. NIST Annual Industrial Fluid Properties Simulation Challenge, AIChE Annual Meeting, Austin, 2002.

1. Aidan Thompson. First Place Prize: Behavior of Polymers in Random Porous Solids). Centennial Graduate Student Research Symposium, University of Pennsylvania, 1993.

POST-DOCTORAL MENTORSHIP

14. Saaketh Desai. Sandia post-doc, 2022-2023. (converted to Sandia technical staff).

13. Andrew Rohskopf. Sandia post-doc, 2022-2023. (Software developer, Boeing Inc.).

12. James Goff. Sandia post-doc, 2021-2022. (converted to Sandia technical staff).

11. Ember McCarthy. Sandia post-doc, 2021-2022. (converted to Sandia technical staff).

10. Ember Sikorski. Sandia post-doc, 2021-2022. (converted to Sandia technical staff).

9. Svetoslav Nikolov. Sandia post-doc, 2020-2021. (converted to Sandia technical staff).

8. Josh Rackers. Truman fellow (co-mentor), 2019-2022. (Research staff, Genetech).

7. Mary Alice Cusentino. Sandia post-doc, 2018-2020. (converted to Sandia technical staff).

6. Julien Tranchida. Sandia post-doc, 2017-2019. (Technical staff, CEA Cadarache, France).

5. Mitchell Wood. Sandia post-doc, 2016-2018. (converted to Sandia technical staff).

4. Tzu-ray Shan. Sandia post-doc, 2011-2015. (Director of Support, Materials Design Inc., San Diego).

3. Saivenkataraman Jayaraman. Sandia post-doc, 2009-2012. (Senior Research Investigator, Bristol-Myers Squibb, New Jersey).

2. Matthew Lane. Sandia post-doc, 2007-2010. (converted to Sandia technical staff).

1. Joanne Budzien. Sandia post-doc, 2008-2010. (X Computational Physics Division, Los Alamos National Laboratory).

STUDENT MENTORSHIP

7. Charlie Sievers. UC Davis. Graduate student intern, 2020-present.
6. Jonathan Wilman. U. South Florida. Doctoral committee, 2019-present.
5. Ashley Williams. U. South Florida. Doctoral committee, 2019-present.
4. Elizabeth Decolvenaere. UC Santa Barbara. Graduate student intern, 2016. (Researcher, D. E. Shaw Research, New York).
3. Tzu-Ray Shan. U. of Florida. Graduate student intern, 2012. (Director of Support, Materials Design Inc., San Diego).
2. Metin Aktulga. Purdue U. Graduate student intern, 2009. (Assistant Professor, Computer Science, Michigan State University).
1. Hansohl Cho. MIT. Graduate student intern, 2008. (Assistant Professor of Aeronautics, Korea Advanced Institute of Science and Technology).

PROFESSIONAL SERVICE

Member-at-Large, DCOMP division, American Physical Society, March (2024)

Session chair, American Physical Society, Minneapolis, March (2024)

Organizing Committee, LAMMPS Workshop and Symposium, Virtual, August (2023)

Session chair, American Physical Society, Las Vegas, March (2023)

Session chair, American Physical Society, Chicago, March (2022)

Organizing Committee, LAMMPS Workshop and Symposium, Virtual, August (2021)

Session chair, American Physical Society, Virtual, March (2021)

Session chair, American Physical Society, Denver, March (2020)

Review Panel, INCITE Program, DOE Leadership Computing, September (2019)

Workshop Chair, LAMMPS Workshop and Symposium, Albuquerque, August (2019)

Session chair, 21st Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter, June (2019)

Minisymposium chair, SIAM Conference on Mathematical Aspects of Materials Science (MS18), July (2018)

Organizing Committee, LAMMPS Workshop and Symposium, Albuquerque, August (2017)

Topic Leader, NSF Workshop on Materials Data, June (2015)

Organizing Committee, LAMMPS Workshop and Symposium, Albuquerque, August (2015)

Session chair, MRS Spring Meeting, San Francisco, March (2014)

Advisory Board, NSF-funded Knowledgebase of Interatomic Potentials (KIM), (2014-present)

Organizing Committee, LAMMPS Workshop and Symposium, Albuquerque, August (2013)

Organizing Committee, LAMMPS Workshop and Symposium, Albuquerque, August (2011)

Organizing Committee, LAMMPS Workshop, Albuquerque, February (2010)

Journal Referee: Physical Review B; Physical Review E; Physical Review Materials; Journal of Chemical Physics; Journal of Physical Chemistry; npj Computational Materials; Nature Communications; Science Advances; Scientific Reports; Computational Materials Science; Modelling and Simulation in Materials Science and Engineering; Journal of Energetic Materials; Journal of Computational Chemistry; Journal of Chemical Theory and Computation

Research Proposal Referee: DOE Basic Energy Science; DOE Office of Fusion Energy; DOE Early Career Award; DOD Multidisciplinary University Research Initiative; Los Alamos National Laboratory LDRD; Sandia National Laboratories LDRD; DOE Early Career Research Program; German Research Foundation; Swiss National Science Foundation

INVITED TALKS

45. Aidan P. Thompson. The LAMMPS particle simulation package: Bringing together innovative physics models, machine-learning interatomic potentials, and extreme-scale computing resources. SIAM Conference on Mathematical Aspects of Materials Science, Pittsburgh, Pennsylvania, May, 2024.

44. Aidan P. Thompson. The LAMMPS particle simulation package: Bringing together innovative physics models, machine-learning interatomic potentials, and extreme-scale computing resources. MRS Spring Meeting, San Francisco, April, 2024.

43. Aidan P. Thompson. The LAMMPS particle simulation package: Bringing together innovative physics models, machine-learning interatomic potentials, and extreme-scale computing resources. Telluride Science Workshop: Machine Learning and Informatics for Chemistry and Materials, Telluride, Colorado, June, 2023.

42. Aidan P. Thompson. The LAMMPS particle simulation package: Bringing together innovative physics models, machine-learning interatomic potentials, and extreme-scale computing resources. Department of Chemistry, Temple U., Philadelphia, Pennsylvania, April, 2023.

41. Aidan P. Thompson. The LAMMPS particle simulation package: Bringing together innovative physics models, machine-learning interatomic potentials, and extreme-scale computing resources. HPC User Forum, Princeton, New Jersey, April, 2023.

40. Aidan P. Thompson. The LAMMPS particle simulation package: Bringing together innovative physics models, machine-learning interatomic potentials, and extreme-scale computing resources. Department of Chemistry, UC Irvine, Irvine, California, April, 2023.

39. Aidan P. Thompson. The LAMMPS particle simulation package: Bringing together innovative physics models, machine-learning interatomic potentials, and extreme-scale computing resources. IPAM Workshop: Increasing the Length, Time, and Accuracy of Materials Modeling Using Exascale Computing, UCLA, Los Angeles, California, March, 2023.

38. Aidan P. Thompson. The LAMMPS particle simulation package: Bringing together innovative physics models, machine-learning interatomic potentials, and extreme-scale computing resources. APS March Meeting, Las Vegas, Nevada, March, 2023.

37. Aidan P. Thompson. The LAMMPS particle simulation package: Bringing together innovative physics models, machine-learning interatomic potentials, and extreme-scale computing resources. Center for Non-linear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico, January, 2023.

36. Aidan P. Thompson. A General Method for Calculating Local Stress and Elastic Constants for Arbitrary Many-body Interaction Potentials in LAMMPS. 10th International Conference on Multiscale Materials Modeling, Baltimore, Maryland, October, 2022.

35. Aidan P. Thompson. SNAP and Beyond: Machine Learning Interatomic Potentials in LAMMPS. Workshop on Multiscale Modeling of Matter under Extreme Conditions, CASUS Institute, Görlitz, Germany, September, 2022.

34. Aidan P. Thompson. Predictive atomistic simulations of materials using SNAP data-driven potentials. CRANN Institute, Department of Physics, Trinity College, Dublin, June, 2022.

33. Aidan P. Thompson. SNAP and Beyond: Machine Learning Interatomic Potentials in LAMMPS. Center for Nonlinear Studies, CNLS Annual Conference 2022 - Physics Informed Machine Learning, Los Alamos National Laboratory, May, 2022.

32. Aidan P. Thompson. SNAP and Beyond: Machine Learning Interatomic Potentials in LAMMPS. Atomic Cluster Expansion Webinar, Ruhr University, Bochum, Germany, 2022.

31. Aidan P. Thompson. High-Fidelity Large-Scale Atomistic Simulations of Materials using LAMMPS, SNAP Interatomic Potentials, and Massively Parallel Computers. Center for Nonlinear Studies Virtual Workshop, Machine Learning in Chemical and Materials Sciences, Los Alamos National Laboratory, May, 2021.

30. Aidan P. Thompson. Predictive atomistic simulations of materials using SNAP data-driven potentials. Center for Computational Science and Engineering, Massachusetts Institute of Technology, Cambridge, February, 2021.

29. Aidan P. Thompson. Introduction to SNAP ML potentials. Molecular Simulation with Machine Learning, Virtual Workshop, Princeton University, July, 2020.

28. Aidan P. Thompson. Machine-learning potentials: The unreasonable effectiveness of linear cluster expansions. Multi-Scale Quantum Mechanical Analysis of Condensed Phase Systems: Methods and Applications, Telluride Science Research Conference, July, 2020.

27. Aidan P. Thompson. Predictive atomistic simulations of materials using snap data-driven potentials in lammps. Physics-Informed Learning Machines for Multiscale and Multiphysics Problems (PhILMs) Webinar, Pacific Northwest National Laboratory, May, 2020.

26. Aidan P. Thompson. Predictive atomistic simulations of materials using SNAP data-driven potentials. American Chemical Society, Philadelphia, April, 2020.

25. Aidan P. Thompson. Prediction of materials properties using SNAP machine-learned interatomic potentials. Artificial Intelligence for Robust Engineering & Science, Oak Ridge National Laboratory, Tennessee, January, 2020.

24. Aidan P. Thompson, Stan Moore, and Rahulkumar Gayatri. Refactoring exaalt md for emerging architectures. Exascale Computing Project Webinar Series, Best Practices for HPC Software Developers, January, 2020.

23. Aidan P. Thompson. Molecular dynamics simulation: Engine of discovery or bridge to nowhere? Computer Science, University of New Mexico, Albuquerque, August, 2019.

22. Aidan P. Thompson. Predictive atomistic simulations of materials using SNAP data-driven potentials. Materials Science Division, Lawrence Livermore National Laboratory, February, 2019.

21. Aidan P. Thompson. Molecular dynamics simulation: Engine of discovery or bridge to nowhere? Information Science and Technology Institute, Los Alamos National Laboratory, June, 2019.

20. Aidan P. Thompson. Predictive atomistic simulations of materials using SNAP data-driven potentials. American Physical Society, Boston, March, 2019.

19. Aidan P. Thompson. Molecular dynamics simulation: Engine of discovery or bridge to nowhere? Plenary Talk, 21st Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter, Portland, June, 2019.

18. Aidan P. Thompson. Predictive atomistic simulations of materials using SNAP machine-learning interatomic potentials. Machine Learning for Computational Fluid and Solid Dynamics conference, Center for Non-Linear Studies, Los Alamos National Laboratory, New Mexico, February, 2019.

17. Aidan P. Thompson. Molecular dynamics simulation: Engine of discovery or bridge to nowhere? Physics, University of South Florida, Tampa, September, 2018.

16. Aidan P. Thompson. Molecular dynamics simulation: Engine of discovery or bridge to nowhere? Chemistry, University of Missouri, Columbia, September, 2018.

15. Aidan P. Thompson. Automated generation of high-accuracy interatomic potentials using quantum data. Artificial Intelligence for Materials Science workshop, National Institute for Standards and Technology, Gaithersburg, August, 2018.

14. Aidan P. Thompson. Automated generation of high-accuracy interatomic potentials using quantum data. SIAM Conference on Mathematical Aspects of Materials Science, July, 2018.

13. Aidan P. Thompson. Atomistic materials simulation using quantum-accurate interatomic potentials. Machine Learning at Interfaces workshop, CECAM-EPFL, Switzerland, June, 2018.

12. Aidan P. Thompson. Automated generation of high-accuracy interatomic potentials using quantum data. TMS Annual Meeting, Phoenix, March, 2018.

11. Aidan P. Thompson. Automated generation of high-accuracy interatomic potentials using quantum data. Machine Learning and Data Science in Materials Modeling, Imaging and Applications, Argonne National Laboratory, May, 2017.

10. Aidan P. Thompson. LAMMPS: A general open-source framework for particle-based simulation of materials on multiple scales. CECAM Workshop on Multiscale Simulation, University College Dublin, Ireland, September, 2016.

9. Aidan P. Thompson. Predictive atomistic simulations of materials using LAMMPS. Tyndall Institute, University College Cork, Ireland, September, 2016.

8. Aidan P. Thompson. Atomistic materials simulation using quantum-accurate interatomic potentials. Machine Learning for Many-Particle Systems, Institute for Pure & Applied Mathematics, UCLA, February, 2015.

7. Aidan P. Thompson. Large-scale atomistic materials simulation using quantum-accurate interatomic potentials. Society of Engineering Science Technical Meeting, Purdue University, Indiana, October, 2014.

6. Aidan P. Thompson. Large-scale atomistic materials simulation using quantum-accurate interatomic potentials. MRS Spring Meeting, San Francisco, March, 2014.

5. Aidan P. Thompson. Large-scale reactive atomistic simulation of shock-induced initiation processes in energetic materials. 18th Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter, Seattle, July, 2013.

4. Aidan P. Thompson. Large-scale atomistic materials modeling using quantum-accurate interatomic potentials. Chemical Engineering, University of New Mexico, Albuquerque, September, 2013.

3. Aidan P. Thompson. Large-scale reactive atomistic simulation of shock-induced initiation processes energetic materials. American Chemical Society, Indianapolis, September, 2013.

2. Aidan P. Thompson. LAMMPS: Overview, timescale acceleration methods, and advanced interatomic potentials. Center For Materials Simulation, Caltech, Pasadena, June, 2011.

1. Aidan P. Thompson. Large scale molecular dynamics simulation using reactive interatomic potentials in LAMMPS. Next Generation Force Fields for Nanoscience workshop, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Tennessee, September, 2010.

PEER-REVIEWED JOURNAL ARTICLES

Over 80 refereed journal articles. Google h-index=37, 9612 citations (3126 in 2023).

Google Scholar: https://scholar.google.com/citations?user=RxtcvuUAAAAJ&hl=en

80. M. A. Cusentino, E. L. Sikorski, M. J. McCarthy, **A. P. Thompson**, and M. A. Wood. Dynamic formation of preferentially lattice oriented, self trapped hydrogen clusters. *Materials Research Express*, 10(10):106513, 2023. doi.

79. M. A. Cusentino, B. Nebgen, K. M. Barros, J. S. Smith, J. D. Shimanek, A. Allen, **A. P. Thompson**, S. J. Fensin, and J. M. D. Lane. Molecular dynamics of high pressure tin phases: Empirical and machine learned interatomic potentials. In *AIP Conference Proceedings*, volume 2844. AIP Publishing, 2023. doi.

78. L. Fiedler, N. A. Modine, S. Schmerler, D. J. Vogel, G. A. Popoola, **A. P. Thompson**, S. Rajamanickam, and A. Cangi. Predicting electronic structures at any length scale with machine learning. *npj Computational Materials*, 9(1):115, 2023. doi.

77. A. Rohskopf, C. Sievers, N. Lubbers, M.A. Cusentino, J. Goff, J. Janssen, M. McCarthy, D. Montes Oca de Zapiain, S. Nikolov, K. Sargsyan, D. Sema, E. Sikorski, L. Williams, **A. P. Thompson**, and M.A. Wood. FitSNAP: Atomistic machine learning with LAMMPS. *Journal of Open Source Software*, 8(84):5118, 2023. doi.

76. J. A. Mitchell, F. F. Abdeljawad, C. C. Battaile, C. Garcia-Cardona, E. A. Holm, E. R. Homer, J. Madison, T. M. Rodgers, **A. P. Thompson**, V. Tikare, E. Webb, and S. Plimpton. Parallel simulation via SPPARKS of on-lattice kinetic and Metropolis Monte Carlo models for materials processing. *Modelling and Simulation in Materials Science and Engineering*, 2023. doi.

75. S. Nikolov, P. Nieves, **A. P. Thompson**, M. A. Wood, and J. Tranchida. Temperature dependence of magnetic anisotropy and magnetoelasticity from classical spin-lattice calculations. *Physical Review B*, 107(9):094426, 2023. doi.

74. E. L. Sikorski, M. A. Cusentino, M. J. McCarthy, J. Tranchida, M. A. Wood, and **A. P. Thompson**. Machine learned interatomic potential for dispersion strengthened plasma facing components. *The Journal of Chemical Physics*, 158(11), 2023. doi.

73. G. Clavier and **A. P. Thompson**. Computation of the thermal elastic constants for arbitrary manybody potentials in lammps using the stress-fluctuation formalism.

72. J. T Willman, K. Nguyen-Cong, A. S. Williams, A. B. Belonoshko, S. G. Moore, **A. P. Thompson**, M. A. Wood, and I. I. Oleynik. Machine learning interatomic potential for simulations of carbon at extreme conditions. *Physical Review B*, 106(18):L180101, 2022. doi.

71. D. Montes de Oca Zapiain, M. A Wood, N. Lubbers, C. Z. Pereyra, **A. P. Thompson**, and D. Perez. Training data selection for accuracy and transferability of interatomic potentials. *npj Computational Materials*, 8(1):189, 2022. doi.

70. **A. P. Thompson**, H. M. Aktulga, R. Berger, D. S. Bolintineanu, W. M. Brown, P. S. Crozier, P. J. in 't Veld, A. Kohlmeyer, S. G. Moore, T. D. Nguyen, R. Shan, M. J. Stevens, J. Tranchida, C. Trott, and S. J. Plimpton. LAMMPS - a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales. *Comp. Phys. Comm.*, 271:108171, 2022. doi.

69. K. Nguyen-Cong, J. T. Willman, Stan G. Moore, A. B. Belonoshko, R. Gayatri, E. Weinberg, M. A. Wood, **A. P. Thompson**, and I. I. Oleynik. Billion atom molecular dynamics simulations of carbon at extreme conditions and experimental time and length scales. In *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis*, Gordon Bell Finalist, SC '21, New York, NY, USA, 2021. Association for Computing Machinery. doi.

68. S. Nikolov, M. A. Wood, A. Cangi, J.-B. Maillet, M.-C. Marinica, **A. P. Thompson**, M. P. Desjarlais, and J. Tranchida. Data-driven magneto-elastic predictions with scalable classical spin-lattice dynamics. *npj Computational Materials*, 7(1):1–12, 2021. doi.

67. Y. Lysogorskiy, C. van der Oord, A. Bochkarev, S. Menon, M. Rinaldi, T. Hammerschmidt, M. Mrovec, **A. P. Thompson**, G. Csányi, C. Ortner, and R. Drautz. Performant implementation of the atomic cluster expansion (PACE) and application to copper and silicon. *npj Computational Materials*, 7(1):97, 2021. doi.

66. J. A. Ellis, L. Fiedler, G. A. Popoola, N. A. Modine, J. A. Stephens, **A. P. Thompson**, A. Cangi, and S. Rajamanickam. Accelerating finite-temperature kohn-sham density functional theory with deep neural networks. *Phys. Rev. B*, 104:035120, Jul 2021. doi.

65. R. Gayatri, S. Moore, E. Weinberg, N. Lubbers, S. Anderson, J. Deslippe, D. Perez, and **A. P. Thompson**. Rapid exploration of optimization strategies on advanced architectures using testsnap and lammps. *arXiv preprint*, 2021. URL `https://arxiv.org/pdf/2011.12875`.

64. M. A. Cusentino, M. A. Wood, and **A. P. Thompson**. Beryllium-driven structural evolution at the divertor surface. *Nuclear Fusion*, 61(4):046049, 2021. doi.

63. J. M. D. Lane, **A. P. Thompson**, I. Srivastava, G. S. Grest, T. Ao, B. Stoltzfus, K. Austin, H. Fan, D. Morgan, and M. D. Knudson. Scale and rate in CdS pressure-induced phase transition. *AIP Conference Proceedings*, 2272(1):100016, 2020. doi.

62. J. T. Willman, A. S. Williams, K. Nguyen-Cong, **A. P. Thompson**, M. A. Wood, A. B. Belonoshko, and I. I. Oleynik. Quantum accurate SNAP carbon potential for MD shock simulations. *AIP Conference Proceedings*, 2272(1):070055, 2020. doi.

61. M.A. Cusentino, M.A. Wood, and **A. P. Thompson**. Suppression of helium bubble nucleation in beryllium exposed tungsten surfaces. *Nuclear Fusion*, 60(12):126018, oct 2020. doi.

60. A. Tran, J. Tranchida, T. Wildey, and **A. P. Thompson**. Multi-fidelity machine-learning with uncertainty quantification and Bayesian optimization for materials design: Application to ternary random alloys. *The Journal of Chemical Physics*, 153(7):074705, 2020. doi.

59. M. A. Cusentino, M. A. Wood, and **A. P. Thompson**. Explicit multielement extension of the spectral neighbor analysis potential for chemically complex systems. *The Journal of Physical Chemistry A*, 124(26):5456–5464, 2020. doi.

58. Y. Zuo, C. Chen, X. Li, Z. Deng, Y. Chen, J. Behler, G. Csanyi, A. V. Shapeev, **A. P. Thompson**, M. A. Wood, and S. P. Ong. Performance and cost assessment of machine learning interatomic potentials. *J. Phys. Chem. A*, 124(4):731–745, 2020. doi.

57. M. A. Wood, M. A. Cusentino, B. D. Wirth, and **A. P. Thompson**. Data-driven material models for atomistic simulation. *Phys. Rev. B*, 99:184305, 2019. doi.

56. J. M. D. Lane, K. Leung, **A. P. Thompson**, and M. E. Cuneo. Water desorption from rapidly-heated metal oxide surfaces-first principles, molecular dynamics, and the Temkin isotherm. *J. Phys.: Condens. Matter*, 30(46):465002, 2018. doi.

55. J. Tranchida, S.J. Plimpton, P. Thibaudeau, and **A. P. Thompson**. Massively parallel symplectic algorithm for coupled magnetic spin dynamics and molecular dynamics. *J. Comp. Phys.*, 372:406 – 425, 2018. doi.

54. M. A. Wood and **A. P. Thompson**. Extending the accuracy of the SNAP interatomic potential form. *J. Chem. Phys.*, 148:241721, 2018. doi.

53. M. A. Wood, D. E. Kittell, C. D. Yarrington, and **A. P. Thompson**. Multiscale modeling of shock wave localization in porous energetic material. *Phys. Rev. B*, 97:014109, 2017. doi.

52. J. M. D. Lane, **A. P. Thompson**, and T. J. Vogler. Enhanced densification, strength and molecular mechanisms in shock compressed porous silicon. *Shocked Compression of Condensed Matter AIP Conference Proceedings*, 1793:120010, 2017. doi.

51. T. R. Shan, R. R. Wixom, and **A. P. Thompson**. Extended asymmetric hot region formation due to shockwave interactions following void collapse in shocked high explosive. *Phys. Rev. B*, 94:054308, 2016. doi.

50. T.-R. Shan, R. R. Wixom, and **A. P. Thompson**. Micron-scale reactive atomistic simulations of void collapse and hotspot growth in petn. *Proceedings 15th International Detonation Symposium ONR-43-280-15*, 2015:962, 2015.

49. T.-R. Shan, R. R. Wixom, and **A. P. Thompson**. Nanoscale void-enhanced initiation in hexanitrostilbene. *Proceedings 15th International Detonation Symposium ONR-43-280-15*, 2015: 878, 2015.

48. **A. P. Thompson**, L. P. Swiler, C. R. Trott, S. M. Foiles, and G. J. Tucker. Spectral neighbor analysis method for automated generation of quantum-accurate interatomic potentials. *J. Comp. Phys.*, 285:316, 2015. doi.

47. C. R. Trott, S. D. Hammond, and **A. P. Thompson**. SNAP: Strong scaling high fidelity molecular dynamics simulations on leadership-class computing platforms. *ISC 2014, Supercomputing, Lecture Notes in Computer Science*, 8488:19, 2014. doi.

46. J. M. D. Lane, **A. P. Thompson**, and T.J. Vogler. Enhanced densification under shock compression in porous silicon. *Phys. Rev. B*, 90:134311, 2014. doi.

45. S. Levy, K. B. Ferreira, **A. P. Thompson**, P. G. Bridges, and C. R. Trott. Evaluating the feasibility of using memory content similarity to improve system resilience. *International Journal of High Performance Computing*, 28:11, 2014. doi.

44. T. Shan and **A. P. Thompson**. Shock-induced hotspot formation and chemical reaction initiation in PETN containing a spherical void. *Journal of Physics: Conference Series*, 500: 172009, 2014. doi.

43. **A. P. Thompson** and T. Shan. Reactive atomistic simulations of shock-induced initiation processes in mixtures of ammonium nitrate and fuel oil. *Journal of Physics: Conference Series*, 500:052046, 2014. doi.

42. T. Shan, A. C. T. van Duin, and **A. P. Thompson**. Development of a ReaxFF reactive force field for ammonium nitrate and application to shock Hugoniots,. *J. Phys. Chem. A*, 118:000, 2014. doi.

41. R. J. Bondi, M. P. Desjarlais, **A. P. Thompson**, G. L. Brennecka, and M. J. Marinella. Electrical conductivity in oxygen-deficient phases of tantalum pentoxide from first-principles calculations. *J. Appl. Phys.*, 114:203701, 2013. doi.

40. S. Root, T. A. Haill, J. M. D. Lane, A. P. Thompson , G. S. Grest, D. G. Schroen, and T. R. Mattsson. Shock compression of hydrocarbon foam to 200 GPa: Experiments, atomistic simulations, and mesoscale hydrodynamic modeling. *J. Appl. Phys.*, 114:103502, 2013. doi.

39. T.-R. Shan, R. R. Wixom, A. E. Mattsson, and **A. P. Thompson**. Atomistic simulation of orientation dependence in shock-induced initiation of pentaerythritol tetranitrate. *J. Phys. Chem. B*, 117:928, 2013. doi.

38. S. J. Plimpton and **A. P. Thompson**. Computational aspects of many-body potentials. *Mat. Res. Soc. Bulletin*, 37:513, 2012. doi.

37. P. L. Theofanis, A. Jaramillo-Botero, W. A. Goddard III, T. R. Mattsson, and **A. P. Thompson**. Electron dynamics of shocked polyethylene crystal. *Phys. Rev. B*, 85:094109, 2012. doi.

36. J. Matthew D. Lane, Gary S. Grest, Aidan P. Thompson, Kyle R. Cochrane, Michael Desjarlais, and Thomas R. Mattsson. Shock compression of hydrocarbon polymer foam using molecular dynamics. *Shocked Compression of Condensed Matter AIP Conference Proceedings*, 1426(1): 1435–1438, 2012. doi.

35. Aidan P. Thompson, J. Matthew D. Lane, and Michael Desjarlais. Molecular dynamics simulation of dynamic response of beryllium. *Shocked Compression of Condensed Matter AIP Conference Proceedings*, 1426(1):1311–1314, 2012. doi.

34. S. Jayaraman, **A. P. Thompson**, and O. A. von Lilienfeld. Molten salt eutectics from atomistic simulations. *Phys. Rev. E*, 84:030201, 2011. doi.

33. H. Asegun, G. Chen, S. J. Plimpton, and **A. P. Thompson**. 1D-to-3D transition of phonon heat conduction in polyethylene using molecular dynamics simulations. *Phys. Rev. B*, 82: 144308, 2010. doi.

32. S. V. Zybin, W. A. Goddard, P. Xu, A. C. T. van Duin, and **A. P. Thompson**. Physical mechanism of anisotropic sensitivity in pentaerythritol tetranitrate from compressive-shear reaction dynamics simulations. *Appl. Phys. Lett.*, 96:081918, 2010. doi.

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