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

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

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

Limited Term Employee
Sandia National Laboratories (Jun. 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

2. Aidan 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.

1. Aidan Thompson. NIST annual industrial fluid properties simulation challenge. First Place Prize (Viscosity of n-nonane/isopropanol mixtures), AIChE Annual Meeting, Austin, November, 2002.

POST-DOCTORAL MENTORSHIP

7. Joshua Rackers. Sandia Truman fellow, 2019-present.
6. Mary Alice Cusentino. Sandia post-doc, 2018-present.
5. Julien Tranchida. Sandia post-doc, 2017-2019. (converted to Sandia technical staff).
4. Mitchell Wood. Sandia post-doc, 2016-2018. (converted to Sandia technical staff).
3. Tzu-ray Shan. Sandia post-doc, 2011-2015. (Director of Support, Materials Design Inc., San Diego).
2. Saivenkataraman Jayaraman. Sandia post-doc, 2009-2012. (Senior Research Investigator, Bristol-Myers Squibb, New Jersey).
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

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; Journal of Chemical Physics; Journal of Physical Chemistry; Science Advances; Scientific Reports; npj Computational Materials; 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; 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

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

24. 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.

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

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

60. Rahulkumar Gayatri, Stan Moore, Evan Weinberg, Nicholas Lubbers, Jack Deslippe, Danny Perez, and **A. P. Thompson**. Optimizing SNAP for future generation architectures using TestSNAP - A proxy app for LAMMPS/SNAP. *Supercomputing 2020*, 1:1, submitted.

59. M. A. Cusentino, Mitchell A. Wood, and **A. P. Thompson**. Explicit multi-element extension of the spectral neighbor analysis potential for chemically complex systems. *accepted J. Phys. Chem. A (arXiv:2003.11570*, 2020. doi.

58. Yunxing Zuo, Chi Chen, Xiangguo Li, Zhi Deng, Yiming Chen, Jorg Behler, Gabor Csanyi, Alexander V. Shapeev, **A. P. Thompson**, Mitchell A. Wood, and Shyue Ping 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.

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.

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.

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. SNAP: Automated generation of quantum-accurate interatomic potentials. *J. Comp. Phys.*, 285:316, 2015.

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.

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.

45. S. Levy, K. B. Ferreira, Bridges P. G. **Thompson**, **A. P.**, 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.

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.

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.

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.

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.

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.

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.

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

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.

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.

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.

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.

31. S. Martin, **A. P. Thompson**, E. A. Coutsias, and J. P. Watson. Topology of cyclo-octane energy landscape. *J. Chem. Phys.*, 132:234115, 2010.

30. W. M. Brown, **A. P. Thompson**, and P. A. Schultz. Efficient hybrid evolutionary optimization of interatomic potential models. *J. Chem. Phys.*, 132:024108, 2010.

29. T. R. Mattsson, J. M. D. Lane, K. R. Cochrane, M. P. Desjarlais, **A. P. Thompson**, F. Pierce, and G. S. Grest. First-principles and classical molecular dynamics simulation of shocked polymers. *Phys. Rev. B*, 81:054103, 2010.

28. S. Jayaraman, **A. P. Thompson**, O. A. von Lilienfeld, and E. J. Maginn. Molecular simulation of the thermal and transport properties of three alkali nitrate salts. *Ind. & Eng. Chem. Res.*, 49:559, 2010.

27. **A. P. Thompson**, S. J. Plimpton, and W. Mattson. General formulation of pressure and stress tensor for arbitrary many-body interaction potentials under periodic boundary conditions. *J. Chem. Phys.*, 131:154107, 2009.

26. J. Budzien, **A. P. Thompson**, and S. V. Zybin. Reactive molecular dynamics simulations of shock through a single crystal of pentaerythritol tetranitrate. *J. Phys. Chem. B*, 113:13142, 2009.

25. **A. P. Thompson**, J. M. D. Lane, M. P. Desjarlais, and M. I. Baskes. Molecular dynamics simulation of dynamic response of beryllium. *Shocked Compression of Condensed Matter AIP Conference Proceedings*, 1195(1):833–836, 2009. doi.

24. J. M. D. Lane and **A. P. Thompson**. Molecular dynamics simulation of shock-induced phase transformation in germanium. *Shocked Compression of Condensed Matter AIP Conference Proceedings*, 1195(1):1157–1160, 2009. doi.

23. A. A. Selezenev, A. Yu. Aleynikov, N. S. Ganchuk, P. V. Ermakov, S. N. Ganchuk, J. B. Aidun, and **A. P. Thompson**. Shock compression calculation of RDX and PETN molecular crystals using Hugoniostat method. *Shocked Compression of Condensed Matter AIP Conference Proceedings*, 1195(1):821–824, 2009. doi.

22. J. Budzien, D. R. Rottach, J. G. Curro, C. S. Lo, and **A. P. Thompson**. A new constitutive model for the chemical aging of rubber networks in deformed states. *Macromolecules*, 41:9896, 2008.

21. A. Slepoy, **A. P. Thompson**, and S. J. Plimpton. A constant-time kinetic Monte Carlo algorithm for simulation of large biochemical reaction networks. *J. Chem. Phys.*, 128:205101, 2008.

20. A. Slepoy, M. D. Peters, and **A. P. Thompson**. Searching for globally optimal functional forms for interatomic potentials using genetic programming with parallel tempering. *J. Comp. Chem.*, 28:2465, 2007.

19. J. Quenneville, T. C. Germann, **A. P. Thompson**, and E. M. Kober. Molecular dynamics studies of thermal induced chemistry in TATB. *Shocked Compression of Condensed Matter AIP Conference Proceedings*, 955(1):451–454, 2007. doi.

18. A. H. Edwards, A. C. Pineda, P. A. Schultz, M. G. Martin, **A. P. Thompson**, H. P. Hjalmarson, and C. J. Umrigar. Electronic structure of intrinsic defects in crystalline germanium telluride. *Phys. Rev. B*, 73:45210, 2006.

17. A. H. Edwards, A. C. Pineda, P. A. Schultz, M. G. Martin, **A. P. Thompson**, and H. P. Hjalmarson. Theory of persistent, p-type, metallic conduction in c-GeTe. *J. Phys.: Cond. Mat.*, 17:329–35, 2005.

16. D. Rottach, J. G. Curro, G. S. Grest, and **A. P. Thompson**. Effect of strain history on stress and permanent set in crosslinking networks: A molecular dynamics study. *Macromolecules*, 37: 5468, 2004.

15. M. G. Martin and **A. P. Thompson**. Industrial property prediction using Towhee and LAMMPS. *Fluid Phase Equilibria*, 217:105, 2004.

14. **A. P. Thompson**. Non-equilibrium molecular dynamics simulation of electroosmotic flow in a charged nanopore. *J. Chem. Phys.*, 119:7503, 2003.

13. M. G. Martin, **A. P. Thompson**, and T. M. Nenoff. Effect of pressure, membrane thickness and placement of control volumes on the flux of methane through thin silicalite membranes. *J. Chem. Phys.*, 114:7174, 2001.

12. M. Chandross, E. B. Webb, G. S. Grest, M. G. Martin, **A. P. Thompson**, and M. W. Roth. Dynamics and exchange at gas-zeolite interfaces i: Pure component butane and isobutane. *J. Phys. Chem. B*, 105:5700, 2001.

11. P. S. Rallabandi, **A. P. Thompson**, and D. M. Ford. A molecular modeling study of entropic and energetic selectivities in air separation with glassy polymers. *Macromolecules*, 33:3142, 2000.

10. L. J. D. Frink, **A. P. Thompson**, and A. G. Salinger. Applying molecular theory to steady-state diffusing systems. *J. Chem. Phys.*, 112:7564, 2000.

9. **A. P. Thompson** and G. S. Heffelfinger. Direct molecular simulation of gradient driven diffusion of large molecules using constant pressure. *J. Chem. Phys.*, 110:10693, 1999.

8. **A. P. Thompson**, D. M. Ford, and G. S. Heffelfinger. Direct molecular simulation of gradient driven diffusion. *J. Chem. Phys.*, 109:6406, 1998.

7. **A. P. Thompson** and E. D. Glandt. Polymers in random porous materials: Structure, thermodynamics and concentration effects. *Macromolecules*, 29:4314, 1996.

6. D. M. Ford, **A. P. Thompson**, and E. D. Glandt. Thermodynamics of fluids in random microporous materials from scaled particle theory. *J. Chem. Phys.*, 103:1099, 1995.

5. **A. P. Thompson** and E. D. Glandt. Adsorption of polymeric fluids in microporous materials. I. Ideal freely-jointed chains. *J. Chem. Phys.*, 99:8325, 1993.

4. **A. P. Thompson**, D. S. Corti, A. L. Myers, and E. D. Glandt. Irreversible adsorption in porous materials. *Fundamentals of Adsorption: Proc. IVth Int. Conf. on Fundamentals of Adsorption.*

3. **A. P. Thompson** and E. D. Glandt. Low coverage kinetics of correlated sequential adsorption. *Phys. Rev. A*, 46:4639, 1992.

2. **A. P. Thompson** and E. D. Glandt. The length of intersection and the number of cusps in assemblies of interpenetrating spheres. *J. Chem. Phys.*, 97:1932, 1992.

1. **A. P. Thompson** and E. D. Glandt. Random sequential adsorption in porous solids. *J. Colloid Interface Sci.*, 146:63, 1991.