Attila Cangi

PERSONAL INFORMATION

Birth place and date	Rotthalmünster, Germany, 29.10.1982
Nationality	German
Languages	German (native), English (full professional proficiency)
Affiliation	Center for Advanced Systems Understanding, Helmholtz-Zentrum Dresden-Rossendorf, Untermarkt 20, 02826 Görlitz
Phone	+49 3581 375 2352
Email	a.cangi@hzdr.de
Web	https://www.ml4md.de
	https://www.casus.science/?page_id=4660

CURRENT POSITION

Head of Department, Center for Advanced Systems Understanding, Helmholtz-Zentrum Dresden-Rossendorf, Germany

SCIENTIFIC CAREER

2024 – now	Helmholtz-Zentrum Dresden-Rossendorf, Germany	Head of Department, Staff Scientist (permanent)
2022 – 2024	Helmholtz-Zentrum Dresden-Rossendorf, Germany	Head of Department (acting), Staff Scientist (permanent)
2020 – 2022	Helmholtz-Zentrum Dresden-Rossendorf, Germany	Staff Scientist
2019 – 2020	Sandia National Laboratories, Albuquerque, USA	Staff Scientist (permanent)
2017 – 2019	Sandia National Laboratories, Albuquerque, USA	Staff Scientist (LTE)
2011 – 2017	Max Planck Institute of Microstructure Physics, Halle (Saale), Germany	Postdoctoral Researcher with E. K. U. Gross

EDUCATION

2006 – 2011	University of California, Irvine, USA	Ph.D., Chemistry with K. Burke
2005 – 2006	Rutgers, The State University of New Jersey, USA	M.Sc., Physics
2001 – 2005	University of Würzburg, Germany	Student, Physics

SUPERVISION AND MENTORING

2020 – now	15 Students (B.Sc. and M.Sc.), 3 Ph.D. Students, 10 Postdocs
2017 – 2020	2 Ph.D. Students, 2 Postdocs
2011 – 2015	1 Ph.D. Student

AWARDS AND HONORS

2023	R&D 100 Award, R&D World, USA
2018	SPOT Award, Sandia National Laboratories, USA

2017	SPOT Award, Sandia National Laboratories, USA
2005 – 2006	German Academic Exchange Service (DAAD) University of Würzburg, Germany and Rutgers, The State University of New Jersey, USA

FUNDING AND PROGRAM MANAGEMENT

PROJECTS AS PRINCIPAL INVESTIGATOR

2021 – 2024	Co-Principal Investigator, Helmholtz AI, *Machine-Learning Based Synthetic Data Generation For Rapid Physics Modeling*, Helmholtz Association, Germany
2019 – 2020	Principal Investigator, Lab Directed Research and Development (Project ID 218454), *Quantum-Accurate Multiscale Modeling of Shock Hugoniots, Ramp Compression Paths, Structural and Magnetic Phase Transitions, and Transport Properties in Highly Compressed Metals*, United States Department of Energy, USA
2017 – 2019	Principal Investigator, Lab Directed Research and Development (Project ID 200202), *Making Density Functionals Work for All Materials*, United States Department of Energy, USA

COLLABORATIVE PROJECTS

2019 – 2022	Lab Directed Research and Development (Project ID 218319), *Accelerating Multiscale Materials Modeling with Machine Learning*, United States Department of Energy, USA
2019 – 2022	Lab Directed Research and Development (Project ID 218456), *Improving Predictive Capability in Radiation, Electrical, and High Energy Density Science Simulations with Fast, Accurate, and Consistent Non-Equilibrium Material Properties*, United States Department of Energy, USA

SCIENCE MANAGEMENT AND INSTITUTIONAL RESPONSIBILITIES

2024 – now	Member of Doctoral Advisory Board, Helmholtz-Zentrum Dresden-Rossendorf, Germany
2022 – now	Member of Working Group *Digitalization*, Helmholtz-Zentrum Dresden-Rossendorf, Germany
2021 – now	Member of Program Committee, Conference Series *Physics of Non-Ideal Plasmas*
2021 – now	Helmholtz AI Associate, Helmholtz Association, Germany
2022 – 2024	Member of Working Group *Graduate student education*, Helmholtz-Zentrum Dresden-Rossendorf, Germany
2018	Coordinator of Summer Student Program, Center for Computing Research, Sandia National Laboratories, USA

ORGANIZATION OF SCIENTIFIC MEETINGS AND SCHOOLS

2024	*Critical Use of AI in Quantum Chemistry, Swiss Chemical Society Seminar on Artificial Intelligence 2024,* University of Fribourg, Switzerland (Member of Organizing Committee)
2023	*Accelerating improvements in Density Functional Theory*, Swiss Federal Institute of Technology, Lausanne, Switzerland (Organization Committee Chair)
2022	*Multiscale Modeling of Matter under Extreme Conditions*, Center for Advanced Systems Understanding, Helmholtz-Zentrum Dresden-Rossendorf, Görlitz, Germany (Program Committee Chair, Local Organizing Committee Chair)
2022	*Strongly Coupled Coulomb Systems*, Center for Advanced Systems Understanding, Helmholtz-Zentrum Dresden-Rossendorf, Görlitz, Germany (Local Organizing Committee Chair, Program Committee Member)
2022	*DFT Methods for Matter under Extreme Conditions,* Center for Advanced Systems Understanding, Helmholtz-Zentrum Dresden-Rossendorf, Görlitz, Germany (Organization Committee Chair)

2019 *Improving the Theory in Density Functional Theory*, Swiss Federal Institute of Technology, Lausanne, Switzerland (Organization Committee Chair)

2018 *Summer Student Program*, Center for Computing Research, Sandia National Laboratories, Albuquerque, USA (Coordinator)

2017 *Teaching the Theory in Density Functional Theory,* Swiss Federal Institute of Technology, Lausanne, Switzerland (Organization Committee Chair)

2016 *Putting the Theory Back in Density Functional Theory,* Institute for Pure and Applied Mathematics, University of California, Los Angeles, USA (Organization Committee Member)

2013 *Density Functional Theory: Learning from the Past, Looking to the Future,* Magnus-Haus of the Deutsche Physikalische Gesellschaft, Berlin, Germany (Organization Committee Member)

INVITED TALKS

2025 Density Functional Theory and Artificial Intelligence Learning from Each Other, CECAM Workshop, Lausanne, Switzerland

2025 Theoretical Chemistry Colloquium, University of Marburg, Germany

2024 Department Seminar, Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

2024 Progress in Ensemble Density Functional Theory: Opportunities and Challenges, Durham University, Durham, United Kingdom

2024 Machine Learning in Electronic-Structure Theory, Institute for Mathematical and Statistical Innovation (IMSI), University of Chicago, USA

2024 APS March Meeting, Focus Session: Big Datasets and Big Data in Physics, Minneapolis, USA

2023 WE-Heraeus Seminar and Max Born Symposium, Many-particles systems under extreme conditions, Görlitz, Germany

2023 Accelerating Improvements in Density Functional Theory, CECAM Workshop, Lausanne, Switzerland

2023 TDDFT School & Workshop: Excited states and dynamics, Rutgers University, Newark, USA

2023 High Energy Density Science Seminar Series, Lawrence Livermore National Laboratory, Livermore, USA

2023 Theoretical Chemistry Seminar, Dresden University of Technology, Germany

2023 Joint Theory Seminar of European XFEL, CFEL, and the University of Hamburg, Germany

2023 Research Seminar Many-Body Theory, Kiel University, Germany

2023 Institute Seminar, Institute of Theoretical Physics, University of Wroclaw, Poland

2022 NHR-Atomistic Simulation Symposium 2022, online, Germany

2022 Research Seminar Many-Body Theory, Kiel University, Germany

2022 Multiscale Modeling of Matter under Extreme Conditions, Center for Advanced Systems Understanding, Helmholtz-Zentrum Dresden-Rossendorf, Görlitz, Germany

2022 Big Data Analytical Methods for Complex Systems, University of Wroclaw, Wroclaw, Poland

2022 International Conference Advanced Systems Research, University of Wroclaw, Wroclaw, Poland

2022 Helmholtz AI Conference 2022, Dresden, Germany

2021 CFEL-DESY Theory Seminar, Hamburg, Germany

2021 8th International Symposium on Optics & its Applications, Rostock, Germany

2021 17th Conference on the Physics of Non-Ideal Plasmas, Dresden, Germany

2021 Supercomputing Frontiers Europe 2021, online

2019	Workshop on the Future of Uncertainty Quantification and Multiscale Modeling Across the Department of Energy, Sandia National Laboratories, Albuquerque, USA
2019	Machine Learning R&D Workshop Sandia National Laboratories, Albuquerque, USA
2019	Z Fundamental Science Workshop, Sandia National Laboratories, Albuquerque, USA
2019	10th International Workshop on Warm Dense Matter, Travemünde, Germany
2019	Computational Modeling for High Energy Density Science and Complex Systems, City University of New York, Department of Physics, New York, USA
2019	Improving the Theory in Density Functional Theory, CECAM Workshop, EPFL Lausanne, Switzerland
2018	Electronic Structure at the Cutting Edge with ELK, MPI of Microstructure Physics, Halle, Germany
2017	Teaching the Theory in Density Functional Theory, CECAM School, EPFL Lausanne, Switzerland
2015	Theoretical Physics Seminar, University of Rostock, Germany
2013	Semiclassical Origins of Density Functionals, Institute for Pure and Applied Mathematics, University of California, Los Angeles, USA
2013	Graduate Student Seminar, Yale University, New Haven, USA

LIST OF PUBLICATIONS

RESEARCH PAPERS

[53] **A. Cangi**, L. Fiedler, B. Brzoza, K. Shah, T. J. Callow, D. Kotik, S. Schmerler, M. C. Barry, J. M. Goff, A. Rohskopf, D. J. Vogel, N. A. Modine, A. P. Thompson, S. Rajamanickam, *Materials Learning Algorithms (MALA): Scalable Machine Learning for Electronic Structure Calculations in Large-Scale Atomistic Simulations*, Comput. Phys. Commun. 314, 109654 (2025).

[52] T. Gawne, Z. A. Moldabekov, O. S. Humphries, K. Appel, C. Baehtz, V. Bouffetier, E. Brambrink, **A. Cangi**, C. Crépisson, S. Göde, Z. Konôpková, M. Makita, M. Mishchenko, M. Nakatsutsumi, L. Randolph, S. Schwalbe, J. Vorberger, U. Zastrau, T. Dornheim and T. R. Preston, *Strong geometry dependence of the X-ray Thomson Scattering Spectrum in single crystal silicon*, Electron. Struct. 7 025002 (2025).

[51] S. Nikolov, K. Ramakrishna, A. Rohskopf, M. Lokamani, J. Tranchida, J. Carpenter, **A. Cangi**, M. A. Wood, *Probing Iron in Earth's Core With Molecular-Spin Dynamics*, Proc. Natl. Acad. Sci. U.S.A. 121, e2408897121 (2024).

[50] K. Ramakrishna, M. Lokamani, **A. Cangi**, *Electrical Conductivity of Warm Dense Hydrogen from Ohm's Law and Time-Dependent Density Functional Theory*, Electron. Struct. 6, 045008 (2024).

[49] **A. Cangi**, *Bridging the gap in electronic structure calculations via machine learning*, Nat. Comput. Sci. 4, 729 (2024).

[48] T. Gawne, H. Bellenbaum, L. B. Fletcher, K. Appel, C. Baehtz, V. Bouffetier, E. Brambrink, D. Brown, **A. Cangi**, A. Descamps, S. Göde, N. J. Hartley, M.-L. Herbert, P. Hesselbach, H. Höppner, O. S. Humphries, Z. Konôpková, A. Laso, B. Lindqvist, J. Lütgert, M. J. MacDonald, M. Makita, W. Martin, M. Mishchenko, Z. A. Moldabekov, M. Nakatsutsumi, J.-P. Naedler, P. Neumayer, A. Pelka, C. Qu, L. Randolph, J. Rips, T. Toncian, J. Vorberger, L. Wollenweber, U. Zastrau, D. Kraus, T. R. Preston, T. Dornheim, *Effects of Mosaic Crystal Instrument Functions on X-Ray Thomson Scattering Diagnostics*, J. Appl. Phys. 136, 105902 (2024).

[47] K. Shah, **A. Cangi**, *Accelerating Electron Dynamics Simulations through Machine Learned Time Propagators*, ICML Workshop 2024, AI for Science: Scaling in AI for Scientific Discovery, arXiv:2407.09628 (2024).

[46] T. Gawne, Z. A. Moldabekov, O. S. Humphries, K. Appel, C. Bähtz, V. Bouffetier, E. Brambrink, **A. Cangi**, S. Göde, Z. Konôpková, M. Makita, M. Mishchenko, M. Nakatsutsumi, K. Ramakrishna, L. Randolph, S. Schwalbe, J. Vorberger, L. Wollenweber, U. Zastrau, T. Dornheim, T. R. Preston,

Ultrahigh resolution x-ray Thomson scattering measurements at the European X-ray Free Electron Laser, Phys. Rev. B 109, L241112 (2024).

[45] H. Tahmasbi, K. Ramakrishna, M. Lokamani, **A. Cangi**, *Machine Learning-Driven Structure Prediction for Iron Hydrides*, Phys. Rev. Mater. 8, 033803 (2024).

[44] V. Martinetto, K. Shah, **A. Cangi**, A. Pribram-Jones, *Inverting the Kohn-Sham equations with physics-informed machine learning*, Mach. Learn.: Sci. Technol. 5 015050 (2024).

[43] T. J. Callow, E. Kraisler, **A. Cangi**, *Physics-enhanced neural networks for equation-of-state calculations*, Mach. Learn.: Sci. Technol. 4, 045055 (2023).

[42] S. L. S. Balakrishnan, M. Lokamani, K. Ramakrishna, **A. Cangi**, D. Murali, M. Posselt, A. A. Sasikala Devi, A. Sharan, *Ab-initio insights on the ultrafast strong-field dynamics of anatase TiO2*, Phys. Rev. B 108, 195149 (2023).

[41] K. Ramakrishna, M. Lokamani, A. Baczewski, J. Vorberger, **A. Cangi**, *Impact of electronic correlations on high-pressure iron: insights from time-dependent density functional theory*, Electron. Struct. 5, 045002 (2023).

[40] L. Fiedler, N. A. Modine, K. D. Miller, **A. Cangi**, *Machine learning the electronic structure of matter across temperatures*, Phys. Rev. B 108, 125146 (2023).

[39] S. Kumar, H. Tahmasbi, K. Ramakrishna, M. Lokamani, S. Nikolov, J. Tranchida, M. A. Wood, **A. Cangi**, *Transferable Interatomic Potentials for Aluminum from Ambient Conditions to Warm Dense Matter*, Phys. Rev. Research 5, 033162 (2023).

[38] L. Fiedler, N. A. Modine, S. Schmerler, D. J. Vogel, G. A. Popoola, A. P. Thompson, S. Rajamanickam, **A. Cangi**, *Predicting electronic structures at any length scale with machine learning*, Npj Comput. Mater. 9, 115 (2023).

[37] T. W. Hentschel, A. Kononov, A. Olmstead, **A. Cangi**, A. D. Baczewski, S. B. Hansen, *Improving dynamic collision frequencies: impacts on dynamic structure factors and stopping powers in warm dense matter*, Phys. Plasmas 30, 062703 (2023).

[36] T. Dornheim, M. P. Böhme, D. Chapman, D. Kraus, T. R. Preston, Z. A. Moldabekov, N. Schlünzen, **A. Cangi**, T. Döppner, J. Vorberger, *Imaginary-time correlation function thermometry: A new, high-accuracy and model-free temperature analysis technique for x-ray Thomson scattering data*, Phys. Plasmas 30, 042707 (2023).

[35] T. Dornheim, Z. A. Moldabekov, K. Ramakrishna, P. Tolias, A. D. Baczewski, D. Kraus, T. R. Preston, D. A. Chapman, M. P. Böhme, T. Döppner, F. Graziani, M. Bonitz, **A. Cangi**, J. Vorberger, *Electronic Density Response of Warm Dense Matter*, Phys. Plasmas 30, 032705 (2023).

[34] K. Ramakrishna, M. Lokamani, A. Baczewski, J. Vorberger, **A. Cangi**, *Electrical Conductivity of Iron in Earth's Core from Microscopic Ohm's Law*, Phys. Rev. B 107, 115131 (2023).

[33] Z. A. Moldabekov, M. Lokamani, J. Vorberger, **A. Cangi**, T. Dornheim, *Non-empirical mixing coefficient for hybrid XC functionals from analysis of the XC kernel*, J. Phys. Chem. Lett. 14, 1326 (2023).

[32] Z. A. Moldabekov, M. Lokamani, J. Vorberger, **A. Cangi**, T. Dornheim, *Assessing the accuracy of hybrid exchange-correlation functionals for the density response of warm dense electrons*, J. Chem. Phys. 158, 094105 (2023).

[31] D. Konar, A. Das Sarma, S. Bhandary, S. Bhattacharyya, **A. Cangi**, V. Aggarwal, *A shallow hybrid classical–quantum spiking feedforward neural network for noise-robust image classification*, Appl. Soft Comput. 136, 110099 (2023).

[30] T. J. Callow, E. Kraisler, **A. Cangi**, *Improved calculations of mean ionization states with an average-atom model*, Phys. Rev. Res. 5, 013049 (2023).

[29] K. Shah, P. Stiller, N. Hoffmann, **A. Cangi**, *Physics-Informed Neural Networks as Solvers for the Time-Dependent Schrödinger Equation*, NeurIPS Workshop Machine Learning and the Physical Sciences (2022).

[28] L. Fiedler, N. Hoffmann, P. Mohammed, G. A. Popoola, T. Yovell, V. Oles, J. A. Ellis, S. Rajamanickam, **A. Cangi**, *Training-free hyperparameter optimization of neural networks for electronic structures in matter*, Mach. Learn.: Sci. Technol. 3, 045008 (2022).

[27] L. Fiedler, Z. A. Moldabekov, X. Shao, K. Jiang, T. Dornheim, M. Pavanello, **A. Cangi**, *Accelerating Equilibration in First-Principles Molecular Dynamics with Orbital-Free Density Functional Theory*, Phys. Rev. Res. 4, 043033 (2022).

[26] M. Schörner, B. B. L. Witte, A. D. Baczewski, **A. Cangi**, R. Redmer, *An ab-initio study of shock-compressed copper*, Phys. Rev. B 106, 054304 (2022).

[25] T. J. Callow, D. Kotik, E. Kraisler, **A. Cangi**, *AtoMEC: an open-source average-atom Python code*, Proceedings of the 21st Python in Science Conference, 37 (2022).

[24] T. Dornheim, P. Tolias, Z. A. Moldabekov, **A. Cangi**, J. Vorberger, *Effective electronic forces and potentials from ab initio path integral Monte Carlo simulations*, J. Chem. Phys. 156, 244113 (2022).

[23] T. J. Callow, E. Kraisler, S. B. Hansen, **A. Cangi**, *First-principles derivation and properties of density-functional average-atom models*, Phys. Rev. Res. 4, 023055 (2022).

[22] L. Fiedler, K. Shah, M. Bussmann, **A. Cangi**, *Deep Dive into Machine Learning Density Functional Theory for Materials Science and Chemistry*, Phys. Rev. Mater. 6, 040301 (2022).

[21] S. Nikolov, J. Tranchida, K. Ramakrishna, M. Lokamani, **A. Cangi**, M. A. Wood, *Dissociating the phononic, magnetic and electronic contributions to thermal conductivity: a computational study in alpha-iron*, J. Mater. Sci. 57, 10535 (2022).

[20] Z. A. Moldabekov, T. Dornheim, G. Gregori, F. Graziani, M. Bonitz, **A. Cangi**, *Towards a Quantum Fluid Theory of Correlated Many-Fermion Systems from First Principles*, SciPost Phys. 12, 062 (2022).

[19] Z. A. Moldabekov, T. Dornheim, J. Vorberger, **A. Cangi**, *Benchmarking Exchange-Correlation Functionals in the Spin-Polarized Inhomogeneous Electron Gas under Warm Dense Conditions*, Phys. Rev. B 105, 035134 (2022).

[18] Z. A. Moldabekov, T. Dornheim, **A. Cangi**, *Thermal Signals from Collective Electronic Excitations in Inhomogeneous Warm Dense Matter*, Sci. Rep. 12, 1093 (2022).

[17] Z. A. Moldabekov, Y. K. Aldakul, N. K. Bastykova, S. Sundar, **A. Cangi**, *Higher harmonics in complex plasmas with alternating screening*, Phys. Rev. Res. 3, 043187 (2021).

[16] S. Nikolov, M. A. Wood, **A. Cangi**, J.-B. Maillet, M.-C. Marinica, A. P. Thompson, M. P. Desjarlais, J. Tranchida, *Data-driven magneto-elastic predictions with scalable classical spin-lattice dynamics*, Npj Comput. Mater. 7, 153 (2021).

[15] Z. A. Moldabekov, T. Dornheim, M. Böhme, J. Vorberger, **A. Cangi**, *The Relevance of Electronic Perturbations in the Warm Dense Electron Gas*, J. Chem. Phys. 155, 124116 (2021).

[14] J. A. Ellis, L. Fiedler, G. A. Popoola, N. A. Modine, J. A. Stephens, A. P. Thompson, **A. Cangi**, S. Rajamanickam, *Accelerating Finite-temperature Kohn-Sham Density Functional Theory with Deep Neural Networks*, Phys. Rev. B 104, 035120 (2021).

[13] T. Dornheim, Z. A. Moldabekov, **A. Cangi**, *A Machine-Learning Surrogate Model for ab initio Electronic Correlations at Extreme Conditions*, ICLR 2021 (2021).

[12] K. Ramakrishna, **A. Cangi**, T. Dornheim, J. Vorberger, *First-principles modeling of plasmons in aluminum under ambient and extreme conditions*, Phys. Rev. B 103, 125118 (2021).

[11] T. Dornheim, **A. Cangi**, K. Ramakrishna, M. P. Böhme, S. Tanaka, J. Vorberger, *Effective static approximation: A fast and reliable tool for warm dense matter theory*, Phys. Rev. Lett. 125, 235001 (2020).

[10] T. Baldsiefen, **A. Cangi**, F. G. Eich, E. K. U. Gross, *Exchange-correlation approximations for reduced-density-matrix-functional theory at finite temperature: Capturing magnetic phase transitions in the homogeneous electron gas*, Phys. Rev. A 96, 062508 (2017).

[9] T. Baldsiefen, **A. Cangi**, E. K. U. Gross, *Reduced-density-matrix-functional theory at finite temperature: Theoretical foundations*, Phys. Rev. A 92, 052514 (2015).

[8] **A. Cangi**, A. Pribram-Jones, *Efficient formalism for warm dense matter simulations*, Phys. Rev. B 92, 161113(R) (2015).

[7] P. Elliott, **A. Cangi**, S. Pittalis, E. K. U. Gross, K. Burke, *Almost exact exchange at almost no computational cost in electronic structure*, Phys. Rev. A 92, 022513 (2015).

[6] R. F. Ribeiro, D. Lee, **A. Cangi**, P. Elliott, K. Burke, *Corrections to Thomas-Fermi Densities at Turning Points and Beyond*, Phys. Rev. Lett. 114, 050401 (2015).

[5] H. Mirhosseini, **A. Cangi**, T. Baldsiefen, A. Sanna, C. R. Proetto, E. K. U. Gross, *Virial theorem and exact properties of density functionals for periodic systems*, Phys. Rev. B 89, 220102(R) (2014).

[4] **A. Cangi**, E. K. U. Gross, K. Burke, *Potential functionals versus density functionals*, Phys. Rev. A 88, 062505 (2013).

[3] **A. Cangi**, D. Lee, P. Elliott, K. Burke, E. K. U. Gross, *Electronic Structure via Potential Functional Approximations*, Phys. Rev. Lett. 106, 236404 (2011).

[2] **A. Cangi**, D. Lee, P. Elliott, K. Burke, *Leading corrections to local approximations*, Phys. Rev. B 81, 235128 (2010).

[1] P. Elliott, D. Lee, **A. Cangi**, K. Burke, *Semiclassical Origins of Density Functionals*, Phys. Rev. Lett. 100, 256406 (2008).

TECHNICAL REPORTS

[7] M. Wood, S. Nikolov, A. Rohskopf, M. P. Desjarlais, **A. Cangi**, J. Tranchida, *Quantum-Accurate Multiscale Modeling of Shock Hugoniots, Ramp Compression Paths, Structural and Magnetic Phase Transitions, and Transport Properties in Highly Compressed Metals*, Technical Report SAND2022-12792, United States Department of Energy (2022).

[6] S. B. Hansen, A. D. Baczewski, T. Gomez, T. W. Hentschel, C. A. Jennings, A. Kononov, T. Nagayama, K. Adler, **A. Cangi**, K. Cochrane, B. Robinson, A. Schleife, *Improving Predictive Capability in REHEDS Simulations with Fast, Accurate, and Consistent Non-Equilibrium Material Properties*, Technical Report SAND2022-13455, United States Department of Energy (2022).

[5] N. A. Modine, J. A. Stephens, L. P. Swiler, A. P. Thompson, J. D. Vogel, L. Fiedler, **A. Cangi**, S. Rajamanickam, *Accelerating Multiscale Materials Modeling with Machine Learning*, Technical Report SAND2022-12875, United States Department of Energy (2022).

[4] J. A. Hubbard, M. A. Omana, D. S. Jensen, **A. Cangi**, T. J. Boyle, *Uranium Aerosol Dynamics: Chemical Kinetics, Primary Particle Formation, Coagulation and Condensation*, Technical Report SAND2019-13154, United States Department of Energy (2019).

[3] **A. Cangi**, F. Sagredo, E. Decolvenaere, A. E. Mattsson, *Semi-local Density Functional Approximations for Bulk, Surface, and Confinement Physics*, Technical Report SAND2019-11805, United States Department of Energy (2019).

[2] **A. Cangi**, *An Exchange-Correlation Functional Capturing Bulk, Surface, and Confinement Physics*, Technical Report SAND2018-7447, United States Department of Energy (2018).

[1] Author list hidden by publisher, Technical Report SAND2017-13554, United States Department of Energy (2017).

EDITED SPECIAL ISSUES AND PROCEEDINGS

[4] J. Yang, **A. Cangi**, A. O. Oliynyk, *Machine Learning and Artificial Intelligence in Materials Science and Condensed Matter Physics*, Materials Today Physics (2025).

[3] S. Vučković, **A. Cangi**, Focus issue: Quantum Chemistry and Artificial Intelligence – learning from each other, Machine Learning: Science and Technology (2024/2025).

[2] **A. Cangi**, J. Citrin, U. von Toussaint (Eds.), *Special issue: Machine learning methods in plasma physics*. Contrib. Plasma Phys. e202300060 (2023).

[1] **A. Cangi**, M. L. Parks, *Center for Computing Research Summer Proceedings 2018*, The Center for Computing Research at Sandia National Laboratories, Technical Report SAND2019-5093R, United States Department of Energy (2019).

BOOK CHAPTERS

[1] L. Fiedler, K. Shah, **A. Cangi**, *Machine-Learning for Static and Dynamic Electronic Structure Theory*. In: Qu, C., Liu, H. (eds) Machine Learning in Molecular Sciences. Challenges and Advances in Computational Chemistry and Physics, vol 36. Springer, Cham (2023).

SOFTWARE PUBLICATIONS

[2] T. J. Callow, D. Kotik, E. Tsvetoslavova Stankulova, N. Rahat, E. Kraisler, **A. Cangi**, *atoMEC* (2023).

[1] **A. Cangi**, S. Rajamanickam, B. Brzoza, T. J. Callow, J. A. Ellis, O. Faruk, L. Fiedler, J. Fox, N. Hoffmann, K. D. Miller, D. Kotik, S. Kulkarni, N. Modine, P. Mohammed, V. Oles, G. A. Popoola, F. Pöschel, J. Romero, S. Schmerler, J. A. Stephens, H. Tahmasbi, A. P. Thompson, S. Verma, D. J. Vogel, *Materials Learning Algorithms (MALA)* (2023).