Curriculum Vitae

Personal Information

Name:	Attila Cangi, Ph.D.
Birth Place and Date:	Rotthalmünster, Germany, 29.10.1982
Nationality:	German
Languages:	German (native), English (full professional proficiency)
ORCID iD:	0000-0001-9162-262X
Institutional Address:	Department Machine Learning for Materials Design, Center for Advanced Systems Understanding, Helmholtz-Zentrum Dresden-Rossendorf, Untermarkt 20, 02826 Görlitz, Germany
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Current Position

Head of Department, Machine Learning for Materials Design, Center for Advanced Systems Understanding, Helmholtz-Zentrum Dresden-Rossendorf, Germany (since 2024)

Academic Career

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, United States	Staff Scientist (permanent)
2017–2019	Sandia National Laboratories, Albuquerque, United States	Staff Scientist (LTE)
2011–2016	Max Planck Institute of Microstructure Physics, Halle (Saale), Germany	Postdoctoral Researcher (with E.K.U. Gross)

Education

2011	University of California, Irvine, United States	PhD in Chemistry (with K. Burke)
2006	Rutgers, The State University of New Jersey, United States	MSc in Physics
2005	University of Würzburg, Germany	*Vordiplom* in Physics

Third-Party Funded Projects

2021–2024	Helmholtz AI, Helmholtz Association	Machine-Learning Based Synthetic Data Generation For Rapid Physics Modeling
2019–2020	DOE, LDRD (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
2019–2022	DOE, LDRD (Project ID 218319)	Accelerating Multiscale Materials Modeling with Machine Learning
2019–2022	DOE, LDRD (Project ID 218456)	Improving Predictive Capability in Radiation, Electrical, and High Energy Density Science Simulations with Fast, Accurate, and Consistent Non-Equilibrium Material Properties
2017–2019	DOE, LDRD (Project ID 200202)	Making Density Functionals Work for All Materials

Awards & Honours

2023	R&D 100 Award, R&D World, United States
2018	SPOT Award, Sandia National Laboratories, United States
2017	SPOT Award, Sandia National Laboratories, United States
2005	German Academic Exchange Service (DAAD), University of Würzburg, Germany and Rutgers, The State University of New Jersey, United States

Academic Service & Leadership

Institutional Responsibilities

2024–present	Member of Doctoral Advisory Board, Helmholtz-Zentrum Dresden-Rossendorf, Germany
2022–present	Member of Working Group *Digitalization*, Helmholtz-Zentrum Dresden-Rossendorf, Germany
2021–present	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, United States

Reviewing Activities

Research Journals	Nature Communications, Nature Computational Science, Nature Communcations Materials, npj Computational Materials, Computer Physics Communications, Scientific Reports, Journal of Chemical Physics, Physical Review Journals, Journal of Physical Chemistry, International Journal of Quantum Chemistry
Funding Agencies	European Research Council (ERC), Swiss National Science Foundation (SNSF), U.S.-Israel Binational Science Foundation (BSF), Centre Européen de Calcul Atomique et Moléculaire (CECAM), National High Performance Computing (NHR)

Supervision & Mentoring

Postdocs supervised:	10
PhD students supervised:	5
MSc/BSc students supervised:	15

Teaching Experience

SS 2025	Nanostructured Materials	Lecture, Exercises	TU Dresden, Germany
WS 2024	Atomistic Simulation Methods	Lecture	TU Dresden, Germany

Memberships

German Physical Society (DPG)

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	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
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 *(selected)*

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, United States
2024	APS March Meeting, Focus Session: Big Datasets and Big Data in Physics, Minneapolis, United States
2023	Accelerating Improvements in Density Functional Theory, CECAM Workshop, Lausanne, Switzerland
2023	TDDFT School & Workshop: Excited states and dynamics, Rutgers University, Newark, United States
2023	High Energy Density Science Seminar Series, Lawrence Livermore National Laboratory, Livermore, United States
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	Big Data Analytical Methods for Complex Systems, 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, United States
2019	Machine Learning R&D Workshop Sandia National Laboratories, Albuquerque, United States
2019	Z Fundamental Science Workshop, Sandia National Laboratories, Albuquerque, United States
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, United States
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

Publications

Research Articles

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, arxiv:2210.12522 (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)](http://doi.org/10.2172/1569522).

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 (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

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).