Chen Shen

Materials Modeling, Ph.D.

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PROFESSIONAL CAREER

University of Wisconsin-Madison — *Madison, US*

Postdoctoral Research Associate — *08. 2023 - 09. 2024*

- Supervisor: Prof. Dr. Dane Morgan and Prof. Izabela Szlufarska

Technische Universität Darmstadt — *Darmstadt, Germany*

Postdoctoral Research Associate — *09. 2022 - 08.2023*

- Supervisor: Prof. Dr. Hongbin Zhang

EDUCATION

Technische Universität Darmstadt — *Darmstadt, Germany*

11. 2018 - 12. 2022

- Supervisor: Prof. Dr. Hongbin Zhang
- Ph.D. Dissertation: Designing Functional Materials Driven by Lattice Degree of Freedom (**Summa Cum Laude**)

Technische Universität Darmstadt — *Darmstadt, Germany*

05. 2015 - 06. 2018

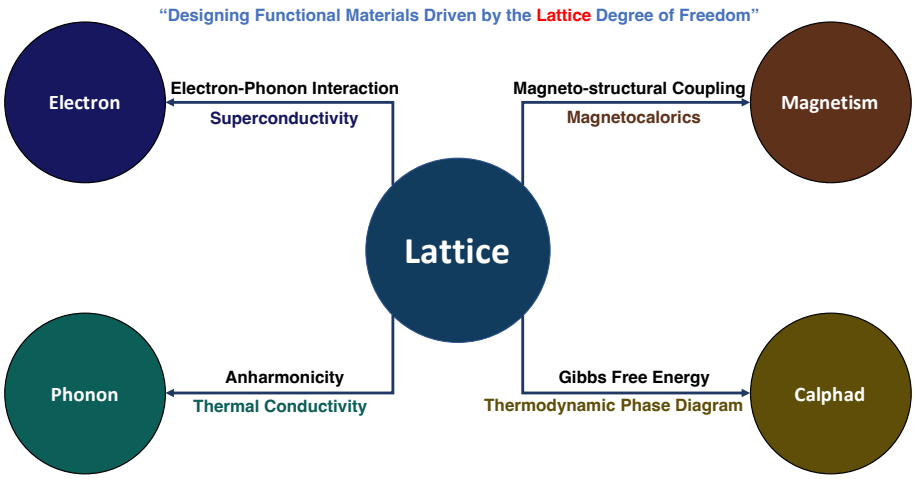
- Supervisor: Prof. Dr. Hongbin Zhang
- Master Thesis: Thermodynamic Assessment of the Magnetic Materials System Supported with First-principles Calculations

Central South University — *Changsha, China*

08. 2010 - 09. 2014

- Supervisor: Prof. Dr. Wenmi Chen
- Bachelor Thesis: Experimental study on flocculants screening test for bauxite washing sludge sedimentation and separation

RESEARCH INTERESTS



During my Ph.D., an integrated paradigm combining the high throughput (HTP), machine learning (ML), and CALculation of PHAse Diagram (CALPHAD) methods was developed to design the functional materials, especially energy materials, including permanent magnets (*e.g.* MAX and MAB phases), magnetocaloric materials (*e.g.* MAB phases), superconductors (*e.g.* $NbSe_2$ and MAX phases), thermoelectric materials (*e.g.* Half-Heusler and 2D materials), thermal management materials (*e.g.* h-BN and Mo_2SiN_4), and low-dimensional catalytic material (*e.g.* Mbene phases). The work focuses on studying the role of the lattice in various interactions, calculating and predicting the properties

resulting from the corresponding couplings (shown in the figure above). In addition, in cooperation with experimental groups, research has also been carried out in phase diagram optimization, high-temperature and high-pressure ceramics, ferroelectrics, negative thermal expansion materials, and optical electronics.

HTP DFT HTP DFT is mainly engaged in designing functional materials and systematically studying the mechanism behind some critical physical phenomena and properties, such as magnetism, mechanics, anharmonicity, and superconductivity.

CALPHAD Combining DFT, the CALPHAD method is used to construct a thermodynamic database, which can be addressed to guide the experimental synthesis of novel functional materials in stable and metastable states.

ML Atomistic models with DFT accuracy can be constructed by developing machine learning interatomic potentials (MLIP) combining HTP calculations and ML.

PROJECT EXPERIENCE

ERC Advanced Grant COOL INNOV

Europe

Main participant of the project *05. 2019 - 05. 2022*

- To accelerate the search for novel and optimized magnetocaloric materials, we performed a high-throughput search for new compounds and detailed calculations of phase transitions from the first principles. In this project, we established an automated HTP workflow for designing functional magnets, which can predict intrinsic magnetic properties, such as magnetic ground state, magnetic anisotropy energy, and transition temperature. Finally, 99 stable magnetic MAB compounds are predicted as potential candidate magnets for magnetocaloric applications.

Fulbright-Cottrell

Germany

Participant of the project *05. 2019 - 01. 2023*

- The aim of this project is to develop a new integrated paradigm to incorporate high throughput DFT calculations, machine learning, and CALPHAD phase diagram, to bridge the gap to multi-scale simulations and to experiments with mutual validation. Hence, I developed such a paradigm and implemented it on the Fe-Sn system.

NOVAMAG: NOVel, critical materials free, high Anisotropy phases for permanent MAGnets, by desin

Germany

Participant of the project *08. 2018 - 09. 2019*

- I participated in this project by contributing to the thermodynamic modeling of phase diagrams. First-principles calculations were carried out to obtain essential parameters, such as mean magnetic moments and transition temperatures, to construct CALPHAD modeling of the magnetic Gibbs energy. The atomic order-disorder transition was considered using the standard cluster variation method. Efficient screening of RE-free uniaxial materials and magnetic characterization could be achieved. MAX and MAB phases as study cases were designed for permanent magnets.

Hessian Competence Center for High-Performance Computing (HKHLR)

Germany

Principal Investigator *2020/2021/2022*

- High Throughput Screening for Novel ternary chalcogenides and binary transition metal nitrides. (Project:00694, 21.1 Mio. core-h)
- Study for external electric field tuned thermal transport properties of two-dimensional materials based on the high throughput density functional theory and machine learning. (Project:01218, 23.3 Mio. core-h)
- High-throughput discovery of MAB and Mbene superconductors. (Project:20160, 17.5 Mio. core-h)

Phadwiki.com

China

Founder *08. 2020 - present*

- Initiated and established the first comprehensive platform for non-profit computing simulation learning exchange in China. Invite many doctors and postdocs in the field of simulation to share knowledge and advanced computing experience, aiming to create a large-scale computing simulation ecological environment suitable for scientific research workers to learn and exchange.

SCHOLARSHIPS & AWARDS

- National Award for Outstanding Self-financed Chinese Students Abroad 2022, China Scholarship Council (CSC)
- TU Darmstadt Award for Outstanding Graduated Thesis (SUMMA CUM LAUDE) (Top 1%)
- TOP STARS Award 2019 （TATA Steel Challenge Award）
- TUDa Scholarship for the international student （2018）
- *Roll student* of Central South University （2014）
- Student Leadership of Central South University （2 times）
- Scholarship of Central South University （3 times）

PUBLICATIONS

(Co[†]-)First-author & Corresponding author[*]

2023	**C. Shen**, TS. Li[*], Y. Zhang, T. Long, M. Dai, J. Shen, C. Wolverton, H. Zhang, Accelerated Screening of Ternary Chalcogenides for Potential Photovoltaic Applications *J. Am. Chem. Soc.*	*J. Am. Chem. Soc.*
2023	K. Hu, R. Xie, **C. Shen[*]**, H. Peng, H. Liu, H. Zhang, High-throughput design of Co-based magnetic Heusler compounds, Acta Mater. 259, 119255.	*Acta Mater.*
2023	H. Wang, Y. Jiao, B. Wu, D. Wang[*], Y Hu, F Liang, **C. Shen[*]**, A Knauer, D Ren[*], H. Wang[*], P. A. Aken, H. Zhang, M. Grätzel, Z. Sofer, P. Schaaf, Exfoliated 2D Layered and Nonlayered Metal Phosphorous Trichalcogenides Nanosheets as Promising Electrocatalysts for CO2 Reduction. *Angew. Chem.*, 2023.	*Angew. Chem.*
2023	S. Lin, **C. Shen[*]**, H. Zhang, Electric-field-tunable thermal conductivity in anti-ferroelectric materials. *Mater. Today Phys.*, 2023.	*Mater. Today Phys.*
2023	**C. Shen**, M. Dai, F. Liang, W. Xie, A. Weidenkaff, T. Tadano[*], H. Zhang[*], Thermal transport properties of $EuTiO_3$: A comparative theoretical and experimental investigation. *Mater. Today Phys.*, (34), 101059.	*Mater. Today Phys.*
2023	R. Yan[†], **C. Shen[†]**, R. Eilhardt, T. Luo, R. Xie, W. Xie[*], M. Widenmeyer, S. Yoon, H. Zhang, A. Weidenkaff, Beneficial contribution of interstitial Cu disorder to electron and phonon transport properties in ZrNiSn half-heusler thermoelectric materials. *Mater. Today Phys.*, in press.	*Mater. Today Phys.*
2023	**C. Shen[†]**, I. Samathrakis[†], K. Hu, HK. Singh, N. Fortunato, H. Liu, O. Gutfleisch, H. Zhang[*], Thermodynamical and topological properties of metastable Fe_3Sn. *Npj Comput. Mater.*, 8, 248.	*Npj Comput. Mater.*
2022	D. Wei, E Zhou, X. Zheng, **C. Shen[*]**, H. Zhang, H. Wang[*], Z. Qin[*], G. Qin[*], Electric-controlled thermal transistor based on Janus monolayer MoSSe. *Npj Comput. Mater.*, 8 (1), 260.	*Npj Comput. Mater.*
2022	MH. Zhang[†], **C. Shen[†]**, CH. Zhao[†], M. Dai, FZ. Yao, B. Wu[*], J. Ma, H. Nan, D. Wang, Q. Yuan, L. Silva, L. Fulanović, A. Schökel, P. Liu, HB. Zhang, JF. Li, N. Zhang[*], K. Wang[*], J. Rödel, M. Hinterstein, Deciphering the phase transition-induced ultrahigh piezoresponse in (K,Na)NbO_3-based piezoceramics. *Nat. Commun.*, 2022, 13, 3434.	*Nat. Commun.*
2022	**C. Shen**, N. Hadaeghi, HK. Singh, T. Long, L. Fan, G. Qin, H. Zhang[*], Two-dimensional bucking structure induces the ultra-low thermal conductivity: A comparative study of the group GaX (X = N, P, As). *J. Mater. Chem. C*, 2022, 10, 1436.	*J. Mater. Chem. C*
2022	**C. Shen**, L. Wang, D. Wei, Y. Zhang, G. Qin[*], X. Chen[*], H. Zhang[*], Novel Two-Dimensional Layered M_2SiN_4 (M = Mo, W): New Promising Thermal Management Materials. *Phys. Chem. Chem. Phys.*, 2022, 24, 3086.	*Phys. Chem. Chem. Phys*
2022	D. Wei, E Zhou, X. Zheng, **C. Shen[*]**, H. Zhang, H. Wang[*], Z. Qin[*], G. Qin[*], Electric-controlled thermal transistor based on Janus monolayer MoSSe. *Npj Comput. Mater.*, 2022, 8, 1.	*Npj Comput. Mater.*
2022	L. Yu, Y. Zhan, D. Wei, **C. Shen[*]**, HB. Zhang, ZZ. Qin[*], GZ Qin[*], Multifunctional two-dimensional graphene-like boron nitride allotrope of g-B_3N_5: A competitor to g-BN? *J. Alloys Compd.*, 2022, 921, 165913.	*J. Alloys Compd.*
2022	B. Li, Y. Yang, H. Qi, Z. Sun, F. Yang, K. Huang, Z. Chen, B. He, X. Xiao, **C. Shen[*]**, N. Wang[*], Monolayer $Sc_2I_2S_2$: An Excellent n-Type Thermoelectric Material with Significant Anisotropy. *ACS Appl. Energy Mater.*, 2022, 6, 7230.	*ACS Appl. Energy Mater.*
2022	H. Qi, Z. Sun, **C. Shen[*]**, C. Zheng, Z. Wang, X. Wang, M. Zhang, N. Wang[*], High thermoelectric performance of monolayer $Al_2X_2Se_2$ (X=Cl, Br, I) with strong anisotropy in lattice thermal conductivity. *ACS Appl. Energy Mater.*, 2022, 5, 7371.	*ACS Appl. Energy Mater.*
2022	Z. Chang, K. Liu, Z. Sun, K. Yuan, S. Cheng, Y. Gao, X. Zhang[*], **C. Shen[*]**, H. Zhang, N. Wang[*], D. Tang[*], First-principles investigation of the significant anisotropy and ultrahigh thermoelectric efficiency of a novel two-dimensional $Ga_2I_2S_2$ at room temperature. *Int. J. Extrem. Manuf.*, 2022, 4, 025001.	*Int. J. Extrem. Manuf.*
2022	Q. Fan, J. Yang, H. Qi, L. Yu, G. Qin, Z. Sun, **C. Shen[*]**, N. Wang[*], Anisotropic thermal and electrical transport properties induced high thermoelectric performance in an $Ir_2Cl_2O_2$ monolayer. *Phys. Chem. Chem. Phys.*, 2022, 24, 11268.	*Phys. Chem. Chem. Phys.*

2022 S. Cheng, Y. He, Z. Chang, Z. Sun, X. Zhang, D. Tang, GK. Li, N. Wang*, **C. Shen***, B. Jiang*, Structural, elastic, phononic, optical and electronic properties investigation of two-dimensional XIS (X=Al, Ga, In) for photocatalytic water splitting. *Int. J. Hydrog. Energy*, 2022, 47, 41640. *Int. J. Hydrog. Energy*

2021 **C. Shen**, Q. Gao, NM. Fortunato, HK. Singh, I. Opahle, O. Gutfleisch, H. Zhang*, Designing of magnetic MAB phases for energy applications. *J. Mater. Chem. A*, 2021, 9, 8805. *J. Mater. Chem. A*

2021 **C. Shen**, K. Hu, L. Fan, H Zhang*, Thermodynamic Reassessment of the Au-In Binary System Supported with First-Principles Calculations. *J. Phase Equilibria Diffus.*, 2021, 42, 479. *J. Phase Equilibria Diffus.*

2021 B. Li, Y. Yang, Z. Sun, H. Qi, Z. Xiong, K. Wu, H. Li, K. Sun, X. Xiao, **C Shen***, N. Wang*, First-Principles Investigation on the Significant Anisotropic Thermoelectric Transport Performance of a Hf_2Cl_4 Monolayer. *J. Phys. Chem. C*, 2021, 126, 525. *J. Phys. Chem. C*

2021 H. Qi, Z. Sun, N. Wang*, G. Qin, H. Zhang, **C. Shen***, Two-dimensional $Al_2I_2Se_2$: A promising anisotropic thermoelectric materials. *J. Alloys Compd.*, 2021, 876, 160191. *J. Alloys Compd.*

2021 Y. Xiao, L. Tang, W. Zhang*, **C. Shen***, Theoretical insights into the selective and activity of CuAu catalyst for O_2 and CO_2 electroreduction. *Comput. Mater. Sci.*, 2021, 192, 110402. *Comput. Mater. Sci.*

2021 L. Fan, **C. Shen***, K. Hu, H. Liu, H. Zhang, DFT Calculations and Thermodynamic Re-Assessment of the Fe-Y Binary System. *J. Phase Equilib. Diffus.*, 2021, 42, 348. *J. Phase Equilib. Diffus.*

2021 Y. Xiao*, **C. Shen***, T. Long, Theoretical Establishment and Screening of an Efficient Catalyst for N_2 Electroreduction on Two-Dimensional Transition-Metal Borides (MBenes). *Chem. Mater.*, 2021, 33, 4023. *Chem. Mater.*

2021 Y. Zhang, **C. Shen***, T. Long, H. Zhang*, Thermal conductivity of h-BN monolayers using machine learning interatomic potential. *J. Phys.: Condens. Matter*, 2021, 33, 105903. *J. Phys.: Condens. Matter*

Co-author

2023 X. Liu*, H. Ding, **C. Shen**, D. Xu, R. Yan, W. Xie*, M. Widenmeyer, E. Ionescu, H. Zhang, A. Weidenkaff, Post-consumer plastics/CoxMn3−xO4 spinels derived Co/MnO@ carbon nanotube composites towards advanced electromagnetic absorbents, *Carbon*, 213, 118273. *Carbon*

2023 YH. Liang, **C. Shen**, H. Liu, C. Wang, D. Li, X. Zhao, LZ. Fan*, Tailoring Conversion-Reaction-Induced Alloy Interlayer for Dendrite-Free Sulfide-Based All-Solid-State Lithium-Metal Battery, *Adv. Sci.*, 2300985. *Adv. Sci.*

2023 A. Rodriguez, C. Lin, **C. Shen**, K. Yuan, M. Al-Fahdi, X. Zhang, H. Zhang, M. Hu*, Unlocking phonon properties of a large and diverse set of cubic crystals by indirect bottom-up machine learning approach, *Commun. Mater.*, 4 (1), 61. *Commun. Mater.*

2023 Y. Xiao*, **C. Shen**, W. Zhang, M. Zhang, H. Zhang, T. Shao, Z Xiong, Y. Ding, L. Liu, Y. Wu*, Comprehensive Study Addressing the Challenge of Efficient Electrocatalytic Biomass Upgrading of 5-(Hydroxymethyl) Furfural (HMF) with a CH3NH2 Ionic Liquid on Metal-Embedded Mo2B2 MBene Nanosheets. *Small*, 2302271. *Small*

2023 Y. Xiao*, **C. Shen**, W. Zhang, M. Zhang, H. Zhang, T. Shao, Z Xiong, Y. Ding, S. Hao, L. Liu, Y. Chen, J. Li*, Electrocatalytic Biomass Upgrading of Furfural using Transition-Metal Borides via Density Functional Theory Investigation. *Small*, 2205876. *Small*

2023 A. Rodriguez, C. Lin, H. Yang, M. Al-Fahdi, **C. Shen**, K. Choudhary, Y. Zhao, J. Hu, B. Cao, H. Zhang, M. Hu*, Million-Scale Atomic Data Integrated Single Deep Neural Network for Predicting Complete Phonon Properties of Heusler Crystals Spanning the Periodic Table. *Npj Comput. Mater.*, 9 (1), 20. *Npj Comput. Mater.*

2022 KC. Zhang*, **C. Shen**, H. Zhang, YF Li, Y Liu, Effect of quartic anharmonicity on the carrier transport of cubic halide perovskites $CsSnI_3$ and $CsPbI_3$. *Phys. Rev. B*, 2022, 106, 235202. *Phys. Rev. B*

2022 A. Rodriguez, C. Lin, H. Yang, M. Al-Fahdi, **C. Shen**, K. Choudhary, Y. Zhao, J. Hu, B. Cao, H. Zhang, M. Hu*, Million-Scale Atomic Data Integrated Single Deep Neural Network for Predicting Complete Phonon Properties of Heusler Crystals Spanning the Periodic Table. *Npj Comput. Mater.*, 2022, accepted. *Npj Comput. Mater.*

2022 HK. Singh, A. Sehrawat, **C. Shen**, I. Samathrakis, I. Opahle, H. Zhang, R. Xie*, High-throughput screening of Half-antiperovskites with a stacked kagome lattice. *Acta Mater.*, 2022, 242, 118474. *Acta Mater.*

2022	I. Samathrakis, N. Fortunato, HK. Singh, **C. Shen**, H. Zhang*, Tunable anomalous hall and nernst effects in MM'X compounds. *J. Phys.: Condens. Matter*, 2022, 51, 025703.	*J. Phys.: Condens. Matter*
2022	A. Reitz, P. Hanna, **C. Shen**, HK. Singh, K. Jayanthi, N. Kubitzaf, A Navrotsky, H. Zhang, U. Wiedwald, C. S. Birkel*, Cr_3GeN: A new nitride with orthorhombic antiperovskite structure. *Chem. Mater*, 2022, 34, 10304.	*Chem. Mater.*
2022	J. Sinclair, J. P. Siebert, M. Juelsholt, **C. Shen**, H. Zhang, and C. S. Birkel*, Facile sol gel-based synthesis of the phosphorus-containing MAX Phase V_2PC. *Inorg. Mater.*, 2022, 61, 16976.	*Inorg. Mater.*
2022	L. Yu, J. Xu, **C. Shen**, E. Zhou, J. Wu, H. Zhang, X. Zheng, H. Wang, G. Qin*, Realizing ultra-low thermal conductivity by the strong synergy of asymmetric geometry and electronic structure in boron nitride and arsenide. *Rare Met.*, 2022, 42, 210.	*Rare Met.*
2022	T. Long, Y. Zhang, NM. Fortunato, **C. Shen**, M Dai, H. Zhang*, Inverse design of crystal structures for multicomponent systems. *Acta Mater.*, 2022, 231, 117898.	*Acta Mater.*
2022	Y. Xiao*, **C. Shen**, Z. Xiong, J. Li*, W. Zhang, A strategy to address the challenge of electrochemical CO_2 and N_2 coupling to synthesis urea on two-dimensional metal borides (MBenes) by computational screening. *Mater. Today Phys.*, 2022, 26, 100726.	*Mater. Today Phys.*
2022	Y. Xiao, **C. Shen**, W. Zhang*, Screening and prediction of metal-doped α-borophene monolayer for nitric oxide elimination. *Mater. Today Chem.*, 2022, 25, 100958.	*Mater. Today Chem.*
2022	Z. Xiong, Y. Xiao*, **C. Shen**, Screening of the Transition Metal Single Atom Anchored on α-Borophene Catalysts as a Feasible Strategy for Electrosynthesis of Urea. *Chem. Mater.*, 2022, 34, 9402.	*Chem. Mater.*
2022	N. Wang, **C. Shen**, Z. Sun, B. Li, H. Xiao*, X. Zu, H. Zhang, Z. Yin, L. Qiao*, Thermal Transport and Mechanical Properties of Layered Oxychalcogenides LaCuOX (X = S, Se, and Te). *ACS Appl. Energy Mater.*, 2022, 5, 6943.	*ACS Appl. Energy Mater.*
2022	E. Zhou, J. Wu, **C. Shen**, H. Zhang, G. Qin*, The stable behavior of low thermal conductivity in 1T-sandwich structure with different components. *J. Appl. Phys.*, 2022, 131, 185702.	*J. Appl. Phys.*
2022	HK. Singh, I. Samathrakis, **C. Shen**, H. Zhang*, Giant anomalous Hall and anomalous Nernst conductivities in antiperovskites and their tunability via magnetic fields. *Phys. Rev. Materials*, 2022, 6, 045402.	*Phys. Rev. Materials*
2022	L. Yu, Y. Tian, X. Zheng, H. Wang, **C. Shen**, G Qin*, Abnormal enhancement of thermal conductivity by planar structure: A comparative study of graphene-like materials. *Int. J. Therm. Sci.*, 2022, 174, 107438.	*Int. J. Therm. Sci.*
2022	F. Duan, **C. Shen**, H. Zhang, G Qin*, Hydrodynamically enhanced thermal transport due to strong interlayer interactions: A case study of strained bilayer graphene. *Phys. Rev. B*, 2022, 105, 125406.	*Phys. Rev. B*
2022	N. Wang, **C. Shen**, Z. Sun, H. Xiao*, H. Zhang, Z. Yin, L. Qiao*, High-Temperature Thermoelectric Monolayer Bi_2TeSe_2 with High Power Factor and Ultralow Thermal Conductivity. *ACS Appl. Energy Mater.*, 2022, 5, 2564.	*ACS Appl. Energy Mater.,*
2021	Y. Xiao*, **C. Shen**, N. Hadaeghi, Transition-Metal Borides (MBenes) as New High-Efficiency Catalysts for Nitric Oxide Electroreduction to Ammonia by a High-Throughput Approach. *Small*, 2021, 17, 2100776.	*Small*
2021	N. Wang, H. Gong, Z. Sun, **C. Shen**, B. Li, H. Xiao*, X. Zu, D. Tang, Z. Yin, X. Wu, H. Zhang, L. Qiao*, Boosting Thermoelectric Performance of 2D Transition-Metal Dichalcogenides by Complex Cluster Substitution: The Role of Octahedral Au6 Clusters. *ACS Appl. Energy Mater.*, 2021, 4, 12163.	*ACS Appl. Energy Mater.*
2021	R. Yan, R. Xie, W. Xie*, **C. Shen**, W. Li, B. Balke, S. Yoon, H. Zhang, A. Weidenkaff, Effects of Doping Ni on the Microstructures and Thermoelectric Properties of Co-Excessive NbCoSn Half-Heusler Compounds. *ACS Appl. Mater. Interfaces*, 2021, 13, 34533.	*ACS Appl. Mater. Interfaces*
2021	Y. Xiao*, **C. Shen**, N. Hadaeghi, Quantum Mechanical Screening of 2D MBenes for the Electroreduction of CO_2 to C1 Hydrocarbon Fuels. *J. Phys. Chem. Lett.*, 2021, 12, 6370.	*J. Phys. Chem. Lett.*
2021	HK. Singh*, I. Samathrakis, NM. Fortunato, J. Zemen, **C. Shen**, O. Gutfleisch, H. Zhang*, Multifunctional antiperovskites driven by strong magnetostructural coupling. *Npj Comput. Mater.*, 2021, 7, 98.	*Npj Comput. Mater.*

2021 T. Long, NM. Fortunato, I. Opahle, Y. Zhang, I. Samathrakis, **C. Shen**, O. Gutfleisch, H. Zhang*, Constrained crystals deep convolutional generative adversarial network for the inverse design of crystal structures. *Npj Comput Mater*, 2021, 7, 66. *Npj Comput. Mater.*

2021 Y. Xiao*, **C. Shen**, Predicted Electrocatalyst Properties on Metal insulator $MoTe_2$ for hydrogen evolution reaction and oxygen reduction reaction application in fuel cells. *Energy Fuels*, 2021, 35, 9, 8275. *Energy Fuels*

2021 KC. Zhang*, L. Cheng, **C. Shen**, Y. Li, Y. Liu, Y. Zhu, Thickness-dependent anisotropic transport of phonons and charges in few-layered $PdSe_2$. *Phys. Chem. Chem. Phys.*, 2021, 23, 18869. *Phys. Chem. Chem. Phys.*

2021 X. Wang, W. Feng, **C. Shen**, Z. Sun, H. Qi, M. Yang, Y. Liu, Y. Wu, X. Wu*, The verification of thermoelectric performance obtained by high-throughput calculations: the case of GeS_2 monolayer from first-principles calculations. *Front. Mater.*, 2021, 8, 709757. *Front. Mater.*

2021 K. Hu, S. Dong, **C. Shen**, H. Liu*, H. Peng, G. Cai, ZP. Jin, Measurement of phase equilibria in Ti-Co-Ge ternary system. *J. Alloys Compd.*, 2021, 793, 653-661. *J. Alloys Compd.*

Under review

2023 LF. Yu, **C. Shen***, GZ, Qin, HB. ZHang, Tuning Thermal Transport Properties by van der Waals Sliding: from Slidetronics to Slidephonics. *Nono Letter*, under review. *Nono Letter*

2023 M. Al-Fahdi, **C. Shen**, C. Lin, K. Yuan, X. Zhang, H. Zhang, M. Hu*, Rapid Prediction of Phonon Density of States by Equivariant Graph Neural Network and High-Throughput Screening of Candidate Substrates for Wide Bandgap Electronic Cooling. *Npj Comput. Mater.*, under review. *Npj Comput. Mater.*

2023 **C. Shen**, R. Xie*, I. Samathrakis, HK. Singh, NM. Fortunato, H. Zhang, Design multifunctional nanolaminated M_2AX (A = V, Cr, Mn, Fe, Co, Ni): Towards permanent magnets and topological properties. *J. Mater. Chem. C*, under review. *J. Mater. Chem. C*

2023 D. Wei, E Zhou, J. Xu, **C. Shen***, H. Zhang, H. Wang*, Z. Qin*, G. Qin*, Stacking-dependent piezoelectric effect on thermal transport in van der Waals two-dimensional materials. *Npj Comput. Mater.*, submitted. *Npj Comput. Mater.*

CONFERENCES & RESEARCH VISITS

Deutsche Physikalische Gesellschaft (DPG) *Regensburg, Germany*

09. 2022

Talk: Self-consistent phonon calculations of lattice dynamical properties

Psi-k 2022 *Lausanne, Switzerland*

08. 2022

Poster: Self-consistent phonon calculations of lattice dynamical properties in cubic $EuTiO_3$ comparing with experimental results

2022 CAMD Summer School *Copenhagen, Denmark*

08. 2022

Poster: Designing Functional Materials Driven by Lattice Degree of Freedom

Virtual Materials Design *Karlsruhe, Germany*

07. 2022

Poster: High-throughput design of magnetic materials

1st China-Germany Meeting on 2D Materials *Mainz, Germany*

04. 2022

Poster: Designing 2D thermoelectric and thermal management materials

APS March Meeting *Online, US*

03. 2021

Talk: Designing of magnetic MAB phases for energy applications

Visting Prof. Zhanpeng Jin's Group *Changsha, China*

11. 2018-02.2019

Invited to visit Prof. Jin's group, guided the students in DFT calculations

Deutsche Physikalische Gesellschaft (DPG) *Dresden , Germany*

03. 2018

Poster: Thermodynamic Assessment of the Magnetic Materials System supported with First-Principles Calculations

TEACHING EXPERIENCE

CALPHAD Lab

TU Darmstadt

Lecturer *Winter Semester 2020/2021/2022*

- Instruct undergraduates to use Thermo-Calc and PyCalphad for thermodynamic calculations and phase diagram optimization.

Quantum Materials Design

TU Darmstadt

Teaching Assistant *Summer Semester 2020/2021*

- Assist in writing course design and teaching plans and guide students on thermodynamic, mechanical, and dynamic stabilities.

Master Thesis

TU Darmstadt

Supervisor *2019 - 2021*

- Supervise eight master students to complete the graduation project calculation and thesis writing. And helped two Chinese postgraduates to achieve the design and writing of CSC proposals.