Yujie Cen

PhD Candidate in Materials Chemistry at TU Wien

Research Interests

My research interests include using first-principles calculations to study the electronic structure and optical properties of materials.

Education

- **PhD in Materials Chemistry**
  TU Wien (July 2023 - Present)
- **MS in Theoretical Physics**
  South China University of Technology (Sept 2020 - July 2023)
- **BS in Physics**
  South China University of Technology (Sept 2016 - July 2020)

Projects

- **PULGON Project**: An initiative focused on understanding Phonons via Line Groups Of Nanomaterials. (https://pulgon-project.org/)

Publications

- Cen, Y., Wieser, S., Madsen, G. K. H., & Carrete, J. (2026). Ab-initio heat transport in defect-laden quasi-1D systems from a symmetry-adapted perspective. *npj Computational Materials, 12*(1), 19.
- Wieser, S., Cen, Y., Madsen, G. K. H., & Carrete, J. (2025). Accelerating first-principles molecular-dynamics thermal conductivity calculations for complex systems. *Journal of Chemical Theory and Computation*.
- Zhu, C., Yan, X., Cen, Y., He, C. C., Zhao, Y. J., & Yang, X. B. (2025). Accelerating the identification of stable configurations in mixed-anion perovskite materials. *Computational Materials Science, 248*, 113564.
- Wieser, S., Cen, Y., Madsen, G. K. H., & Carrete, J. (2025). Accelerating Green-Kubo heat transport simulations for quasi-1D systems using highly accurate machine-learned force fields. *PSI-K 2025: abstracts book*.

- Li, D. Z., Cen, Y., Wang, X., & Yang, X. B. (2024). Residual entropy of ice: A study based on transfer matrices. *Physical Review B, 110*(19), 195414.
- Li, D. Z., Cen, Y., Wang, X., & Yang, X. B. (2024). Residual Entropy of Hexagonal Ice and Cubic Ice: A Transfer Matrix Description. *arXiv e-prints, arXiv:2404.13897*.
- Xiong, J., Peng, Y. H., Lin, J. Y., Cen, Y., Yang, X. B., & Zhao, Y. J. (2023). High Concentration Intrinsic Defects in MnSb2Te4. *Materials, 16*(15), 5496.
- Cen, Y., He, C. C., Qiu, S. B., Zhao, Y. J., & Yang, X. B. (2022). Determining ground states of alloys by a symmetry-based classification. *Physical Review Materials, 6*(5), L050801.
- Lin, J. Y., Chen, Z. J., Li, G. L., Zeng, J., Cen, Y., et al. (2022). Theoretical study of magnetic phase transition in La23M13MnO3 (M= Ca, Sr) membranes through strain and doping. *Physics Letters A, 432*, 128010.