

Shishir Kumar PANDEY

Publications

Published

- 2025 **Anomalous magnetism in 3d-4f double perovskite oxide with Kramers' ion**, Saurav Kumar, Shantanu Majumder, Francesco Congiu, Giuseppe Muscas, H. Luetkens, S. D. Kaushik, Shishir K. Pandey, Stephen L. Lee, Uday Deshpande, Tapati Sarkar, Soumya Jyoti Ray, (Accepted in Phys. Rev. B.)
- 2025 **Half-metallicity and wandering axis ferromagnetism in Mn substituted Fe_2TiSn** , Kulbhushan Mishra, Shishir Kumar Pandey, S Chaudhuri, Rajiv Rawat, PA Bhobe, (Accepted in Phys. Rev. B.), Link: <https://arxiv.org/abs/2407.11576>
- 2025 **Electron spectroscopy study of single crystal CrTe**, A. R. Shelke, C. N. Kuo, Shishir Kumar Pandey, T. L. Nguyen, Y. X. Chen, Y. T. Cheng, F. H. Chang, M. Yoshimura, N. Hiraoka, T. W. Pi, H. J. Lin, C. T. Chen, A. Fujimori, Priya Mahadevan, C. S. Lue, and A. Chainani, **Phys. Rev. B**, 111, 085142, <https://doi.org/10.1103/PhysRevB.111.085142>
- 2025 **Learning local equivariant representations for quantum operators**, Zhanghao Zhouyin, Zixi Gan, Shishir Kumar Pandey, Linfeng Zhang, Qiangqiang Gu, (Accepted in ICLR 2025), <https://openreview.net/forum?id=kpq3lljUD3>
- 2024 **Computational exploration of a viable route to Kitaev-quantum spin liquid phase in OsCl_3** , Qiangqiang Gu, Shishir Kumar Pandey[†], Yihao Lin, **Phys. Rev. Res.**, 6 (4), 043309, Link: <https://doi.org/10.1103/PhysRevResearch.6.043309> ([†] corresponding author)
- 2024 **Pitfalls of Exchange-Correlation Functionals in Descriptions of Magnetism: Cautionary Tale of the FeRh Alloy**, Shishir Kumar Pandey[†], Saikat Debnath, Zhanghao Zhouyina, Qiangqiang Gu, **Com. Mat. Sci.**, 248, 113561, <https://doi.org/10.1016/j.commatsci.2024.113561>
- 2024 **DeePTB: A deep learning-based tight-binding approach with *ab initio* accuracy**, Qiangqiang Gu, Zhanghao Zhouyin, Shishir Kumar Pandey, Peng Zhang, Linfeng Zhang, Weinan E, **Nat. Comm.**, 15 (1), 6772, Link: <https://www.nature.com/articles/s41467-024-51006-4>
- 2024 **Terahertz crystal electric field transitions in a Kondo-lattice antiferromagnet**, Payel Shee, Chia-Jung Yang, Shishir Kumar Pandey, Ashis Kumar Nandy, Ruta Kulkarni, Arumugam Thamizhavel, Manfred Fiebig, and Shovon Pal, **Phys. Rev. B**, 109 (7), 075133, <https://journals.aps.org/prb/abstract/10.1103/PhysRevB.109.075133>
- 2023 **A computational method to estimate spin-orbital interaction strength in solid state systems**, Qiangqiang Gu, Shishir Kumar Pandey[†] and Rajarshi Tiwari, **Compt. Mat. Sci.**, 221, 112090, Link: <https://doi.org/10.1016/j.commatsci.2023.112090> ([†] corresponding author)
- 2023 **Emergence of bond-dependent highly anisotropic magnetic interactions in Sr_4RhO_6 : a theoretical study**, Shishir Kumar Pandey[†], Qiangqiang Gu, Yihao Lin, Rajarshi Tiwari and Ji Feng, **Phys. Rev. B**, 107, 115119, Link: <https://doi.org/10.1103/PhysRevB.107.115119> ([†] corresponding author)
- 2022 **Spin interaction and magnetism in cobaltate Kitaev candidate materials: An *ab initio* and model Hamiltonian approach**, Shishir Kumar Pandey and Ji Feng, **Phys. Rev. B**, 106, 174411, Link: <https://doi.org/10.1103/PhysRevB.106.174411>
- 2022 **Charge doping to flat AgF_2 monolayers in a chemical capacitor setup**, Daniel Jezierski, Adam Grzelak, Xiaoqiang Liu, Shishir Kumar Pandey, Maria N. Gastiasoro, José Lorenzana, Ji Feng and Wojciech Grochala, **Phys. Chem. Chem. Phys.** 24, 15705–15717, Link: <https://doi.org/10.1039/D2CP00179A>

- 2022 **Microscopic origin of room-temperature ferromagnetism in the double perovskite $\text{Sr}_2\text{FeReO}_6$** , *Shishir Kumar Pandey, Ashis K. Nandy, Poonam Kumari, and Priya Mahadevan*, **Phys. Rev. B** 105, 214422, Link: <https://doi.org/10.1103/PhysRevB.105.214422>
- 2022 **Silver(II) route to unconventional superconductivity**, *Xiaoqiang Liu**, *Shishir Kumar Pandey**, and *Ji Feng*, **Phys. Rev. B** 105, 134519, Link: <https://doi.org/10.1103/PhysRevB.105.134519> (* equal contribution)
- 2021 **Understanding the ferromagnetic insulating state in Cr-doped VO_2 : Density functional and tight binding calculations**, *Shishir Kumar Pandey, Abhinav Kumar, Sagar Sarkar, and Priya Mahadevan*, **Phys. Rev. B** 104, 125110, Link: <https://doi.org/10.1103/PhysRevB.104.125110>
- 2021 **Dynamical correlation enhanced orbital magnetization in Vl_3** , *Zhimou Zhou, Shishir Kumar Pandey, and Ji Feng*, **Phys. Rev. B** 103, 035137, Link: <https://doi.org/10.1103/PhysRevB.103.035137>
- 2020 **Site substitution in GdMnO_3 : Effects on structural, electronic, and magnetic properties**, *Sudipta Mahana, Shishir Kumar Pandey, Bipul Rakshit, Pronoy Nandi, Raktima Basu, Sandip Dhara, S. Turchini, N. Zema, U. Manju, Subhendra D. Mahanti, and D. Topwal*, **Phys. Rev. B** 102, 245120, Link: <https://doi.org/10.1103/PhysRevB.102.245120>
- 2020 **Probing the Electronic Structure of Hybrid Perovskites in the Orientationally Disordered Cubic Phase**, *Pronoy Nandi*, S. K. Pandey*, Chandan Giri, Vijay Singh, L. Petaccia, U. Manju, Subhendra D. Mahanti, and D. Topwal*, **J. Phys. Chem. Lett.** 11, 14, 5719, Link: <https://doi.org/10.1021/acs.jpclett.0c01386> (* equal contributions)
- 2020 **Layer-Dependent Electronic Structure Changes in Transition Metal Dichalcogenides: The Microscopic Origin**, *Shishir K. Pandey, Ruma Das, and Priya Mahadevan*, **ACS Omega** 5, 25, 15169, Link: <https://doi.org/10.1021/acsomega.0c01138>
- 2019 **Effect of boundary scattering on spin-hall effect**, *Shishir K. Pandey†, Tribhuvan P. Pareek*, **Euro. Phys. B** 92,131, Link: <https://doi.org/10.1140/epjb/e2019-90501-8> († corresponding author)
- 2019 **Recent progress in physical effects of Berry phase in condensed matter systems**, *Lu Zhuocheng, PANDEY Shishir Kumar, Ji Feng*, **Science Foundation in China** 3, Link: <https://www.cnki.com.cn/Article/CJFDTotat-ZJJJ201903046.htm>
- 2017 **Doping an antiferromagnetic insulator: A route to an antiferromagnetic metallic phase**, *Shishir K. Pandey, Priya Mahadevan and D. D. Sarma*, **EuroPhys. Lett.** 117, 57003, Link: <https://doi.org/10.1209/0295-5075/117/57003>
- 2016 **Driving force for martensitic transformation in $\text{Ni}_2\text{Mn}_{1+x}\text{Sn}_{1-x}$** , *Soumyadipta Pal, Sagar Sarkar, S. K. Pandey, Chhayabrita Maji, and Priya Mahadevan*, **Phys. Rev. B** 94, 115143, Link: <https://doi.org/10.1103/PhysRevB.94.115143>
- 2012 **Route to high Néel temperatures in 4d and 5d transition metal oxides**, *S. Middey, Ashis Kumar Nandy, S. K. Pandey, Priya Mahadevan, and D. D. Sarma*, **Phys. Rev. B** 86, 104406, Link: <https://doi.org/10.1103/PhysRevB.86.104406>

Under active consideration/Preprints/In-communication/In-preparation

- 2025 **Emergence of a hidden-order phase well below the charge density wave transition in a topological Weyl semimetal**, *Sk Kalimuddin, Sudipta Chatterjee, Arnab Bera, Satyabrata Bera, Deep Singha Roy, Soham Das, Tuhin Debnath, Ashis Kumar Nandy, Shishir K. Pandey† Mintu Mondal*, In communication with Adv. Func. Mat.
- 2023 **The driving force for charge ordering in rare earth nickelates**, *Basudeb Mandal, Sagar Sarkar, Shishir Kumar Pandey, Priya Mahadevan, Cesare Franchini, A.J. Millis, D.D. Sarma*, In communication with Phys. Rev. Lett., Link: <https://arxiv.org/abs/1701.06819v1>
- 2023 **Synopsis of Co-based materials as possible candidates for Kitaev physics**, *Shishir Kumar Pandey, Ji Feng*, Manuscript in-preparation
- 2023 **Absence of insulator to metal transition at higher band fillings: A model Hamiltonian study**, *Shishir Kumar Pandey and Priya Mahadevan*, Manuscript in-preparation

- 2023 **Fermi surface instability and sliding charge density waves (CDWs) in the quasi one-dimensional quantum material $(\text{TaSe}_4)_2\text{I}$** , *Sk Kalimuddin, S. K. Pandey, Ashis K. Nandi, and Mintu Mondal*, Manuscript in-preparation (communicating author)
- 2023 **Fate of anisotropic magnetic interactions in quasi-one dimensional spin chains in face-shared geometry: The case of $\text{K}_3\text{Ir}_2\text{O}_6$** , *S. K. Pandey*, Manuscript in-preparation