Max-Planck-Institut für
Struktur und Dynamik der Materie

Max Planck Institute for the Structure and Dynamics of Matter

IMPRS UFAST Call for PhD applications 2024/2025

AR4 - Unraveling Microscopic Origins of Phase Transition in Excitonic Insulator C Machine Learning Force Fields

Title of PhD Project	**Unraveling Microscopic Origins of Phase Transition in Excitonic Insulator Candidates with Machine Learning Force Fields**
Type	Theory
Supervisor(s)	Prof. Angel Rubio, Dr. Burak Gurlek, Dr. Simone Latini, Dr. Mariana Rossi,
Affiliation(s):	Max Planck Institute for the Structure and Dynamics of Matter
Number of positions:	1
Abstract:	The excitonic insulator (EI) is an exotic phase of matter that rises from the spontaneous formation of an excitonic bound state in semiconductors or semi-metals, and their condensation [1-2]. This phase holds potential for important implications such as superfluid energy transport, making it a topic of immense interest in condensed matter physics. Despite its theoretical significance, the EI phase has not been conclusively observed in real materials, largely due to the complex interplay of electronic and structural instabilities in candidate materials like Ta_2NiSe_5 [1-3]. In this project, we aim to shed light on the microscopic origin of experimentally observed phase transition in EI candidate materials. The project will focus on one of the missing pieces of the puzzle: the study of structural phase transition [1]. Using ab initio molecular dynamics (MD) simulations, we will investigate the anharmonic phonon-phonon coupling mechanism to reveal the role of phononic instabilities in the phase transition. To access realistic dynamics, we will employ state-of-the-art machine learning techniques to enhance the capabilities of ab initio MD [4]. This project will also involve collaborations with the leading international experimental groups. [1] L. Windgätter, M. Rösner, G. Mazza, H. Hübener, A. Georges, A. J. Millis, S. Latini, and A. Rubio. Common microscopic origin of the phase transitions in Ta_2NiSe_5 and the excitonic insulator candidate Ta_2NiSe_5, *Npj Comput. Mater.* 7, 210 (2021). [2] E. Baldini, A. Zong, D. Choi, C. Lee, M.H. Michael, L. Windgaetter, I.I. Mazin, S. Latini, D. Azoury, B. Lv, A. Kogar, Y. Su, Y. Wang, Y. Lu, T. Takayama, H. Takagi, A.J. Millis, A. Rubio, E. Demler, N. Gedik. The spontaneous symmetry breaking in Ta_2NiSe_5 is structural in nature, *Proc. Natl. Acad. Sci.*, 120 (17) (2023).

	[3] J. Huang, B. Jiang, J. Yao, D. Yan, X. Lei, J. Gao, Z. Guo, F. Jin, Y. Li, Z. Yuan, et al. Evidence for an Excitonic Insulator State in $Ta_2Pd_3Te_5$, *Phys. Rev. X*, 14, 011046 (2024). [4] I. Batatia, D. P. Kovacs, G. Simm, C. Ortner, and G. Csányi, Mace: Higher order equivariant message passing neural networks for fast and accurate force fields. Adv. Neural Inf. Process. Syst., 35, 11423–11436 (2022).
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