Talk information

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Title of the talk: Informatics-enabled quantum materials design

Abstract of the talk:

The rapid progress in informatics techniques, particularly in algorithms and machine learning, has significantly accelerated the discovery of quantum materials. Notably, ferroelectrics and superconductors have found extensive applications such as information storage, magnetic resonance imaging, and magnetic levitation trains. However, the quest for robust nanoscale ferroelectrics and high critical temperature superconductors remains a challenge. Aim in addressing these limitations, this presentation will showcase our recent endeavors in the application of informatics-enabled crystal structure prediction methods to design novel oxides that exhibit strongest ferroelectricity at only 1 nanometer up to date (Science, 379, 6638, 2023). In addition, I will discuss the applications of high-throughput structure screening and machine learning into the predictions of high-temperature superconducting hydrides. The experimentally reported but retracted work (Nature 615, 244, 2023) by the team of Ranga Dias on the room-temperature superconductivity in Lu-H-N systems at 1 GPa will be discussed. Despite the retraction, I will talk about the reasons responsible for the absence of room-temperature superconductivity at 1 GPa, and the potential implementation of high-temperature and room-temperature superconductivity at moderate and high pressures due to the quantum effect (arXiv:2307.10699, 2023). On top of it, we propose over 50 ambient-pressure superconducting hydrides. One of these hydrides exhibits a superconducting temperature of 80 K, exceeding the critical temperatures of existing hydrides, which are typically lower than 10 K at ambient pressure. Our prediction invites the world-wide experimental groups to validate the superconductivity in this hydride (arXiv:2310.06804, 2023).

Biography of the speaker:

Yue-Wen Fang, currently a postdoc at the University of the Basque Country, is set to transition into a tenured scientist at the Spanish National Research Council (CSIC) in Fall 2024. Before relocating to Spain, he held researcher positions at the Tokyo Institute of Technology and Kyoto University. He has coauthored 2 book chapters, and 47 scientific papers including publications in prestigious journals such as Science, Nature Communications, and Advanced Materials. His research primarily focuses on the theoretical design of information materials, energy materials, and superconducting materials. Dr. Fang has served as a referee for 24 peer-reviewed journals and the Horizon European grant, and the Youth Editor of Acta Metallurgica Sinica (English Letters).