Semiconductor Defect Physics for Energy Materials: From First Principles to Machine Learning

Point defects are prevalent in semiconductors and fundamentally control their electronic and optoelectronic properties. In photovoltaic materials, they govern non-radiative recombination losses that limit power conversion efficiency, but identifying the microscopic origin of these losses remains non-trivial. In this talk, I will present two complementary computational approaches developed around antimony selenide (Sb_2Se_3), an emerging earth-abundant photovoltaic material whose efficiency has plateaued at around 10% despite a decade of experimental progress.

First, I will introduce a framework for predicting trap-limited conversion efficiency that can take input from either theoretical simulations or experimental measurements [1]. By incorporating defect concentrations and carrier capture cross-sections, we go beyond the textbook Shockley–Queisser limit and predict a realistic upper efficiency of 26% for Sb_2Se_3 under optimal growth conditions [2]. This approach also allows us to identify the dominant recombination centres and suggests possible strategies, such as defect passivation, to mitigate their impact.

Second, I will discuss how machine learning interatomic potentials (MLIPs) can accelerate defect simulations by orders of magnitude. Current foundation MLIPs fail for charged point defects, where local bonding environments deviate strongly from the pristine bulk. We address this by incorporating global charge embeddings within the MACE architecture and adopting a multi-fidelity training strategy that combines semi-local and hybrid density functional theory reference data [3]. The resulting force fields reproduce defect structures and energetics in quantitative agreement with hybrid density functional theory calculations at a fraction of the cost, enabling large-scale exploration of defect physics in semiconductors.

References:

[1] https://github.com/WMD-group/TrapLimitedConversion

[2] Wang X, Kavanagh S R, Scanlon D O, et al. Upper efficiency limit of Sb_2Se_3 solar cells. Joule, 2024, 8(7): 2105-2122.

[3] Wang X, Mosquera-Lois I, Walsh A. Multi-fidelity Machine Learning Interatomic Potentials for Charged Point Defects. arXiv preprint arXiv:2603.05238, 2026.