Accelerating point defect photo-emission calculations with machine-learning interatomic potentials

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We introduce a computational framework leveraging universal machine learning interatomic potentials (MLIPs) to dramatically accelerate the calculation of photoluminescence (PL) spectra of atomic or molecular emitters with ab initio accuracy. By replacing the costly density functional theory (DFT) computation of phonon modes with much faster MLIP phonon mode calculations, our approach achieves speed improvements exceeding an order of magnitude with minimal precision loss. We benchmark the approach using a dataset comprising ab initio emission spectra of 791 color centers spanning various types of crystal point defects in different charge and magnetic states. The method is also applied to a molecular emitter adsorbed on a hexagonal boron nitride surface. Across all the systems, we find excellent agreement for both the Huang-Rhys factor and the PL lineshapes. This application of universal MLIPs bridges the gap between computational efficiency and spectroscopic fidelity, opening pathways to high-throughput screening of defect-engineered materials. Our work not only demonstrates accelerated calculation of PL spectra with DFT accuracy, but also makes such calculations tractable for more complex materials.

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