Unveiling the evolution of charge density wave order in twisted bilayers of $NbSe_2$: A Machine-Learning approach

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Niobium diselenide has garnered significant interest over the past decade due to the coexistence of superconductivity and a charge density wave (CDW), which have been experimentally observed down to the monolayer limit. Their coexistence, and evolution with varying numbers of layers and different twisting angles are central topics in twistronics and would benefit from accurate atomistic simulations. However, traditional first-principles methods fall short due to the large number of atoms needed to accommodate the long-wavelength moiré pattern. This study adopts a practical approach by leveraging ab initio data to develop accurate machine learning interatomic potentials thanks to the ALLEGRO architecture, an open-source code for building highly scalable and accurate equivariant deep learning interatomic potentials. We explore the formation and evolution of CDW order in monolayers and twisted bilayers. Our results are validated against density functional theory calculations, encompassing structural relaxation and phonon dispersions, with minimal errors observed in energy and forces.