“Visualizing ultrafast lattice dynamics at 2D van der Waals interfaces using ultrafast electron diffraction”

Charge and energy transfer processes at the junction of atomically thin, two dimensional (2D) materials are an area of burgeoning interest because van der Waals crystals allow for the creation of arbitrary, atomically precise heterostructures simply by stacking disparate monolayers without the constraints of covalent bonding or epitaxy. At a type II heterojunction between two 2D semiconductors, ultrafast charge transfer has been previously determined to occur on the order of 10’s of femtoseconds after photoexcitation. However, the coupling between the lattice degrees of freedom of the photoexcited monolayers remains less understood. We use ultrafast electron diffraction to directly visualize lattice dynamics in the individual monolayers of the van der Waals heterojunction. Here, we use mega-electronvolt ultrafast electron diffraction (MeV-UED) to directly visualize lattice dynamics in photoexcited heterostructures of WSe2/WS2 monolayers. Following selective optical excitation of WSe2, we uncover surprisingly strong thermal coupling between WSe2 and WS2, leading to nearly concurrent heating of both layers on picosecond timescales. This equilibration occurs at a rate orders of magnitude faster than what is explained by vibrational coupling alone. With the aid of first principles calculations, we are able to shed light on the role of lattice dynamics during ultrafast electronic processes at 2D van der Waals heterojunctions. Taken together, our work indicates strong electron-phonon coupling via layer-hybridized electronic states – a powerful route to control energy transport across atomic junctions.