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Exploring ultrafast dynamics in photoexcited layered materials by large-scale quantum molecular dynamics simulations[1] ARAVIND KRISHNAMOORTHY, CACS, USC, LINDSAY BASSMAN, CACS, Dept. of Physics Astronomy, AIICHIRO NAKANO, RAJIV KALIA, PRIYA VASHISHTA, CACS, Depts. of Physics Astronomy, Computer Science, and Chemical Engg. and Material Science, USC, HIROYUKI KUMAZOE, MASAAKI MISAWA, FUYUKI SHIMOJO, Dept. of Physics, Kumamoto University — Understanding ultrafast dynamics in photoexcited few-layer transition metal dichalcogenide crystals is crucial for synthesis and functionalization of these materials. These dynamics also hold the key to unraveling phenomena such as anisotropic thermal transport and anomalous lattice expansion. But, a thorough investigation of such dynamics requires computationally-demanding *ab initio* methods to capture electron-phonon interactions as well as a laterally-large simulation cells to account for long-range vibrational modes that are not sampled in small-scale DFT calculations. Here, we present results from our non-adiabatic QMD simulations of mono and few-layer TMDCs at experimentally-realized sub-μm length scales, made possible through our linear-scaling DFT method. We discuss how large-scale simulations allow us to model phenomena like electron-lattice coupling, correlated atomic motion and localized configurational change and address recent experimental observations in these material systems.

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Aravind Krishnamoorthy
CACS, USC

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