Tuning Thermal Transport in Transition Metal Dichalcogenide Monolayers and Heterostructures

Amalya C. Johnson[1]
Johnathan D. Georgaras[1], Xiaozhe Shen[2], Helen Yao[1,2], Ashley P. Saunders[3], Helen J. Zeng[3], Hyungjin Kim[3], Aditya Sood[4], Tony F. Heinz[2,4,5], Aaron M. Lindenberg[1,4,6], Duan Luo[1,2], Felipe H. da Jornada[1], Fang Liu[3]
[1] *Department of Materials Science and Engineering, Stanford University, Sanford, CA 94305, USA*
[2] *SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA*
[3]*Department of Chemistry, Stanford University, Sanford, CA 94305, USA*
[4]*Stanford Institute for Materials and Energy Science, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA*
[5]*Department of Applied Physics, Stanford University, Stanford CA 94305*
[6]*Stanford PULSE Institute, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA*
amalyaj@stanford.edu

Monolayer and heterobilayer transition metal dichalcogenides (TMDCs) are of particular interest for tuning materials properties and studying emergent physical phenomena due to their enhanced excitonic effects, spin-valley polarization, and anisotropic thermal conductivities. Here, we study thermal transport in TMDC heterostructures and monolayers using Ultrafast Electron Diffraction (UED), Raman spectroscopy, and Time-Domain Thermoreflectance (TDTR). Using UED, we studied the photoexcited phonon dynamics and interfacial thermal transport properties in MoS_2/WS_2 and $WSe_2/MoSe_2$ twisted heterobilayers and their dependence on twist angle. We identified an interlayer heat transfer channel with a characteristic timescale of ~20 picoseconds, about one order of magnitude faster than molecular dynamics simulations assuming initial intralayer thermalization. Atomistic calculations involving phonon-phonon scattering suggest that this process originates from the nonthermal phonon population following the initial interlayer charge transfer and scattering [1]. We use Raman and TDTR to measure the thermal conductivity of strained monolayer TMDCs and identify new methods to tune thermal transport in these materials. This work reveals the nature of heat transport in TMDC monolayers and heterostructures and will aid in the thermal management of their device applications in the future.

References

[1] A. C. Johnson, J. D. Georgaras, X. Shen, H. Yao, A. P. Saunders, H. J. Zeng, H. Kim, A. Sood, T. F. Heinz, A. M. Lindenberg, D. Luo, F. H. da Jornada, F. Liu. *Science Advances* **10**, eadj8819 (2024).

Figures

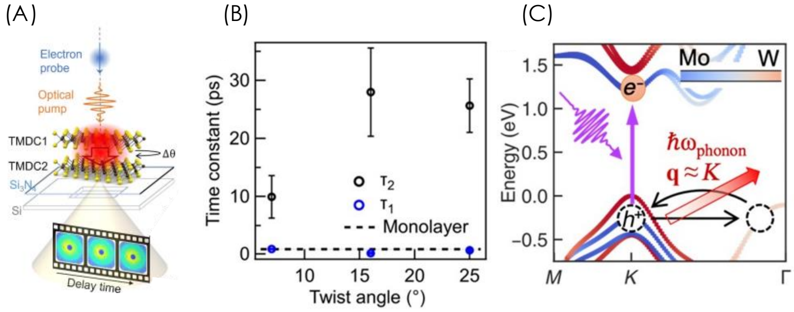

Figure 1: (a) UED visualizes lattice dynamics in TMDC heterobilayers (b) The rate of heat transfer between layers is identified at different twist-angles (c) First-Principles calculations reveal phonon scattering channel driving heat transfer.