2D Crystal Consortium
NSF Materials Innovation Platform

PennState
Materials Research Institute

The Pennsylvania State University, N-338 Millennium Science Complex, University Park, PA 16802

MIP: 2D Crystal Consortium
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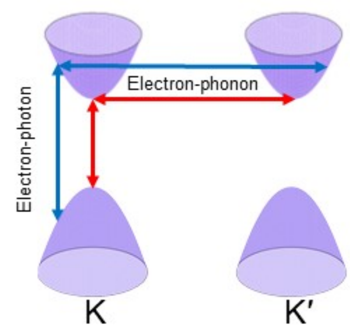
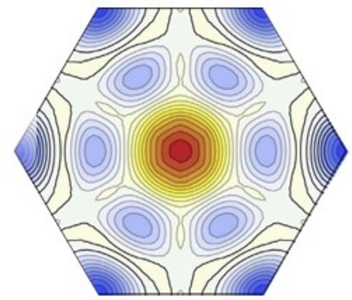
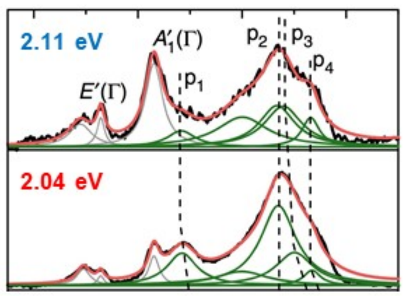
Unveiling intervalley scattering in 2D crystals

Light and lattice vibrations in a crystal do not interact strongly in general, but both interact strongly with electrons. This three-way interaction allows a characterization method known as double resonance Raman spectroscopy to map out the low-energy electronic structure of materials and assign vibrational signatures to different microscopic processes. Double resonance in two-dimensional MoS_2 reveals the dynamics of excitons – robust elementary excitations of a 2D crystal – between two sets of low-energy states known as valleys. The accurate assignment of vibrational signatures elucidates the essential physics limiting the performance of a novel class of “valleytronic” devices exploiting the selectivity of valleys to incident light carrying different polarizations.







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NSF DMR DIVISION OF MATERIALS RESEARCH
DIRECTORATE FOR MATHEMATICAL AND PHYSICAL SCIENCES

Carvalho, Wang, Mignuzzi, Roy, Terrones, Fantini, Crespi, Malard, Pimenta, Universidade Federal de Minas Gerais, Penn State, King’s College London

Figure Title: Vibrational Responses in Molybdenum Disulfide.

Figure Caption: The energies of electrons in monolayer MoS2 is shown to determine the link between two types of interactions: electron with light, and electron with lattice vibrations. For example, the lower panel shows two different vibrational responses when the material is excited with light at different wavelengths.

What Has Been Achieved: A family of longstanding mis-assignments of Raman signatures in 2D transition metal dichalcogenides has been corrected by the collaboration between double resonance Raman spectroscopy experiments and first-principles calculations. Selection rules for intervalley scattering processes in MoS_2 have been derived from group theory and verified from first-principles.

Importance of Achievement: The study establishes the dominance of LA(K) phonons in intervalley scattering, a process responsible for the destruction of valley polarization, thus highlighting the need for controlling this phonon mode for future efforts on valleytronic devices.

Unique Features of the MIP That Enabled Project: Close collaboration between synthesis, characterization, and theory efforts.

Publication: B. R. Carvalho, Y. Wang, S. Mignuzzi, D. Roy, M. Terrones, C. Fantini, V. H. Crespi, L. M. Malard, and M. A. Pimenta, “Intervalley scattering by acoustic phonons in two-dimensional MoS2 revealed by double-resonance Raman spectroscopy”, Nat. Commun. 8, 14670 (2017).