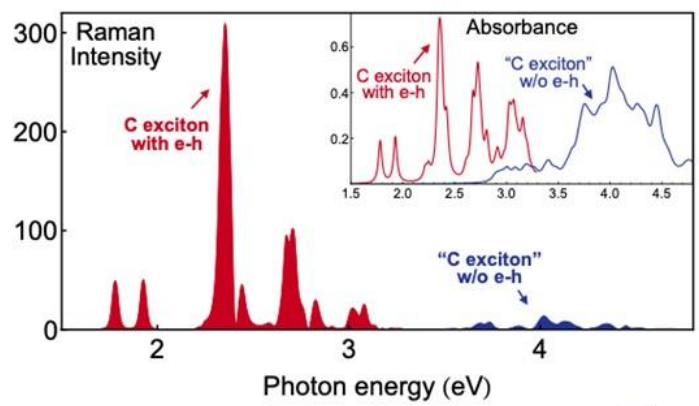
MIP: 2D Crystal Consortium
DMR-1539916

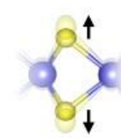
2018

# Strong exciton regulation of Raman scattering

One of the most useful ways that materials interact with light is Raman scattering, in which a photon creates or absorbs a lattice vibration. When the photon energy equals an electronic transition in the material (a "resonance"), the scattering can become much stronger. An outstanding mystery in 2D transition metal dichalcogenides has been the pronounced weakness of some excitonic resonances compared to others. The 2DCC-MIP team has developed an efficient first-principles way to calculate excitonic resonant Raman intensities, thereby explaining the puzzling near-absence of resonant Raman response around the A and B excitons (band-edge excitations with very strong optical absorption) and the pronounced strength of the resonant Raman response from the C exciton (which arises from parallel valence and conduction bands). These insights can now be carried to other semiconducting systems.




The so-called "C exciton" resonance appears very strongly in full Raman intensity calculation (red), but is much weaker in a calculation that omits excitonic effects (blue). The efficient perturbative approach used here also opens up the method to much more complex systems and high-throughput data-intensive modes of analysis.



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**What Has Been Achieved:** A new highly efficient method to calculate resonant Raman intensities including excitonic effects.

**Importance of Achievement:** This new method allows us to better interpret and utilize high-throughput optical characterization of 2D materials, including potential roles of defects and heterostructures. This could be enabling of data-intensive modes of analysis and allows us to access new routes towards understanding electron-phonon interactions.

**Unique Features of the MIP That Enabled Project:** The 2DCC-MIP mission of pushing the state-of-the-art in advanced characterization of 2D materials.

**Publications:** Y. Wang, B. R. Carvalho, and V. H. Crespi, "Strong exciton regulation of Raman scattering in monolayer $MoS_2$", Phys. Rev. B **98**, 161405(R).

The 2DCC-MIP is funded by NSF cooperative agreement DMR-1539916.