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Electron-phonon interactions in transition metal dichalcogenides

Effects of doping and valley structure

Thursday May 20th, 2021 – 16.00

Online streaming using Google Meet
Link: https://meet.google.com/yud-upbp-mno

Speaker

Thibault SOHIER – University of Liège (Belgium)

Abstract

Owing to the multi-valley and spin-textured nature of their electronic structure, semiconducting transition-metal dichalcogenides (TMDs) offer the possibility for a combined manipulation of charge, spin, and valley degrees of freedom, leading to fascinating fundamental physics and technological prospects. Charge, spin and valley transport all depend on the scattering of carriers by phonons. In parallel, further control of those degrees of freedom is often achieved via electrostatic doping.
Thus, it is essential to understand the interplay between electronic structure, doping and electron-phonon interactions in TMDs. Density functional theory and analytical models are used to build an extensive and predictive model of electron-phonon scattering as a function of valley structure and doping.
Intervalley scattering depends on doping mostly via the position of the Fermi level with respect to the different valleys and the associated energy selection rules. Intravalley scattering, however, displays a rather complex doping dependency via two kinds of electronic screening depending on the phonon perturbation. The first is the standard free carrier screening which reduces the coupling as carrier density increases. In contrast, the second surprisingly leads to an enhanced electron-phonon interaction at high doping, when multiple valleys are occupied. The impact of those mechanisms on the physical properties of TMDs is illustrated by computing the mobility of semiconducting TMDs and showing large variations as a function of doping and valley structure.

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