First–principles investigations of lattice dynamics of chosen transition metal dichalcogenides systems

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Recently, group VI-B transition metal dichalcogenides (TMDCs) attract significant interest due to their extraordinary and tunable electronic and optical properties [1, 2]. Their quasi two-dimensional character leads to the anisotropy of their physical properties, which has various technological applications. Moreover, the mixed layered crystals allow for continuous tuning of the optical bandgap, rendering the TMDCs alloys the appealing materials for applications in electronic and optoelectronic devices. Hence, an experimental characterization and theoretical analysis of the properties of mixed crystals is of fundamental importance. This work is focused on the phonon properties of chosen TMDC systems, especially the influence of composition variations in mixed crystals.

We study from first principles (DFT) dynamical properties of several MX_2 bulk crystals and monolayers (M=Mo; X=S, Se). Dynamical properties of $MoS_{2(1-x)}Se_{2x}$ alloys are investigated within a supercell model for different compositions x. We check the influence of van der Waals corrections to DFT. The calculated phonon dispersions and densities of states reproduce well the measured Raman spectra [3]. We are able to explain the evolution of Raman modes by analysing the projected phonon density of states at Γ point of reciprocal space. Additionally, we develop a phonon vector unfolding technique at the center of the Brillouin zone [4]. It simplifies the crowded supercell phonon dispersions and allows for a direct comparison with experimental data.

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