Simulation of Phonon Spectra in Three-Component Two-Dimensional Crystals of Refractory-Metal Dichalcogenides

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Abstract / Аннотация: A model for ab initio calculation of the phonon properties of three-component solid solutions of refractory-metal dichalcogenides was developed based on the assumption that displacements of the same type of chalcogen atoms and decoupled displacements of the metal atoms were identical. The calculated phonon frequencies at the Γ-point for monomolecular layers of MoS2–xSex and MoS2–xTex agreed with existing experimental Raman spectra.

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