Select the right atom to adjust atomic motions in transition metal dichalcogenides

Transition Metal Dichalcogenides (TMDs) are materials made from sheets of transition metal cations (Mo, W etc.) sandwiched between two sheets of chalcogen atoms (S, Se, Te); such atomic sandwiches are held together by weak forces (e.g. van der Waals), yelding a lamellar (layered) structure (Fig. 1).

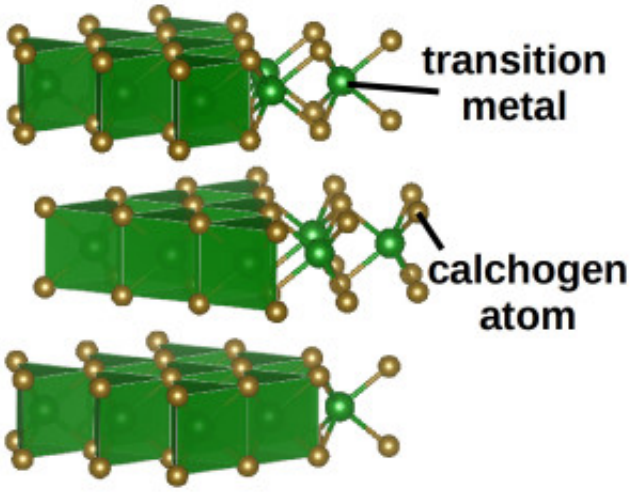

Fig. 1. Lamellar structure of a generic transition metal dichalcogenide material.

Their peculiarities open several routes to achieve unprecedented properties of wide applicability, such as in photovoltaic devices, lithium ion batteries, hydrogen evolution catalysis, transistors, photodetectors, DNA detection, memory devices and tribological applications. In addition to their versatile chemical composition and stoichiometry, dimensionality plays a key role in determining the characteristics of TMDs. When produced as thin films formed by a finite number of layer n, intrinsic atomic motions (e.g. vibrational modes) become important either for the structural response to external stimuli, either during synthesis processes. The study of such motions at the atomic scale becomes thus mandatory for their use in nanoengineered materials.

We used computer simulations (within the Density Functional Theory) to study how the number of layers and the kind of atom determine the atomic motions intrinsic of the system. We find that the electronic distribution in the interlayer region is crucial to determine the frequencies of the motions. Therefore, to tune such frequencies, it is enough to adjust the electron density. This is possible by a proper substitution of the atoms forming the structure. The main issue is that the frequency/electron density/atomic type relation is not trivial and it is not easy to pick the right atom from the periodic table.

To overcome this difficulty, we focused on all the possible pair of atoms forming the system and elaborated a way (metric) to measure how such couple contributes to form the overall atomic motions. We call “cophonicity” this way to characterize the atomic pair. Using the cophonicity, we know how to select the proper atomic type to tune the structural frequencies at a fixed number of layers. This is important in those applications where the number of layers must be kept fixed, while preserving the electronic characteristics of the chosen TMD material.

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