Finite temperature vibrational and thermal properties of Dichalcogenides

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Interest in the transition metal dichalcogenide materials has exploded due to their wide range of physical properties, which go from photovoltaic to thermoelectric applications. Dichalcogenides are also known to have a low out of plane thermal conductivity due to their layered structures. We present the vibrational and thermal properties of different Dichalcogenides,calculated using the Temperature Dependent Effective Potential package, linked as a library with Abinit, to calculate the finite temperature lattice dynamics. In particular we use an efficient automatic scheme for generating distorted snapshots which allows us to calculate anharmonic effects avoiding long ab-initio molecular dynamics runs.