A Comparative Phonon and Phonon Transport Properties of Some Bulk and Two Dimensional Materials

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The research on graphene despite some serious drawbacks motivated the researchers to explore other two dimensional (2D) materials. The 2D materials are one of the most active areas of nanomaterials research due to their far reaching potential applications. So far monolayer of hexagonal boron nitride (h-BN), silicine, transition metal chalcogenides, phosphorene and many other have been synthesized or predicted. A significant impact for the development of nanodevices and nanoelectronics has been gathered by these 2D materials due to their astonishing electrical, optical and mechanical properties. The 2D materials are one-atom thick honeycomb lattice of elements and compounds. While most of the works on these 2D materials focus on the electronic properties, the recent studies focus on the phonon studies mainly to reveal whether monolayer honeycomb structures possess local minima on the Born-Oppenheimer surface. Furthermore, the transport properties of the materials play an important role in their applications. For application in thermoelectric energy (TE) conversion, one requires low lattice thermal conductivity of material simultaneously maintaining the high value of electrical conductivity. The TE figure of merit of ZT can be improved by optimizing the geometry size to decrease the lattice thermal conductivity. Thus systematic investigation of phonon transport properties for 2D materials is needed for which a detail phonon studies is essential.

In this presentation, we report on density functional theory (DFT) simulations aiming to understand the phonon and phonon transport properties of two classes of materials, selected IV-VI mono-chalcogenides and boron nitride (BN) in bulk as well as 2D forms. The focus lies on the phonon dispersion of these two different classes of materials. While in the case of IV-VI chalcogenides, we have studied not only the phonon properties of GeSe and GeTe with pressure for selected three pressure dependent phases but also in 2D structure. A complete analysis of phonon dispersion curves and thermoelectric properties will be provided in context of structure and dimension. The other material which we choose is the haeckelite BN (heck-BN) sheet a material similar to the h-BN sheet, the second most important material in the 2D materials category after graphene. The heck-BN sheet is a new form of structure in 2D, demonstrated based on the presence of square-octagonal pair in BN monolayer grown on Cu (111) surface. We discuss phonon dispersion curve and phonon transport properties of heck-BN and compare with other BN nanostructure including bulk BN.