replacing MAR17-2016-006451

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Machine learnt bond order potential to investigate the low thermal conductivity of stanene nanostructures MATHEW CHERUKARA, BADRI NARAYANAN, ALPER KINACI, KIRAN SASIKUMAR, STEPHEN GRAY, MARIA CHAN, SUBRAMANIAN SANKARANARAYANAN, Argonne Natl Lab — The growth of stanene on a Bi_2Te_3 substrate has engendered a great deal of interest, in part due to stanene's predicted exotic properties. In particular, stanene shows promise in topological insulation, large-gap 2D quantum spin hall states, lossless electrical conduction, enhanced thermoelectricity, and topological superconductivity. However, atomistic investigations of growth mechanisms (needed to guide synthesis), phonon transport (crucial for designing thermoelectrics), and thermo-mechanical behavior of stanene are scarce. This paucity is primarily due to the lack of inter-atomic potentials that can accurately capture atomic interactions in stanene. To address this, we have developed a machine learnt bond-order potential (BOP) based on Tersoff's formalism that can accurately capture bond breaking/formation events, structure, energetics, thermodynamics, thermal conductivity, and mechanical properties of single layer tin, using a training set derived from density functional theory calculations. Finally, we employed our newly developed BOP to study anisotropy in thermal conductivity of stanene sheets, temperature induced rippling, as well as dependence of anharmonicity and thermal conductivity on temperature.

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Date submitted: 11 Nov 2016 Electronic form version 1.4