Structural Stability & Electronic properties of IV-VI thin Nanowires

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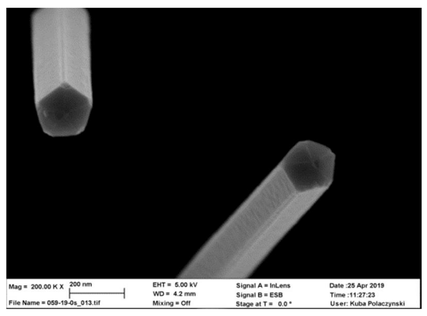
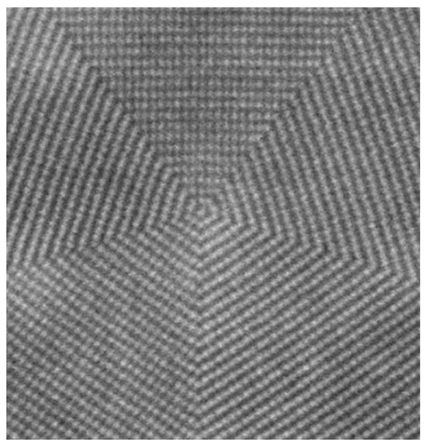
ABSTRACT

We used density functional theory to study the electronic properties and structural stability of thin SnTe and PbTe cubic nanowires (CNs) and pentagonal nanowires (PNs) grown along [001] and [110] directions. The band structures illustrated a trivial insulating behavior for thin CNs, while the bands connecting valence and conduction electrons are observed for thin PNs within a trivial band structure. We estimated that topological band structure is expected in SnTe CNs for thicknesses larger than 13 nm, and we can assume a similar value for the PNs. The bands connecting valence and conduction electrons in thin PNs mainly originate from the central atom as observed from partial charge density making the disclination responsible for band crossing and thus metallicity. Moreover, the binding energies revealed that the stability increases as the thickness of nanowires increases and CNs are more stable than PNs. In addition, the absence of imaginary phonons modes in the phonon spectra indicate the dynamical stability of CNs and PNs. Therefore, the PNs are in a metastable structural phase.

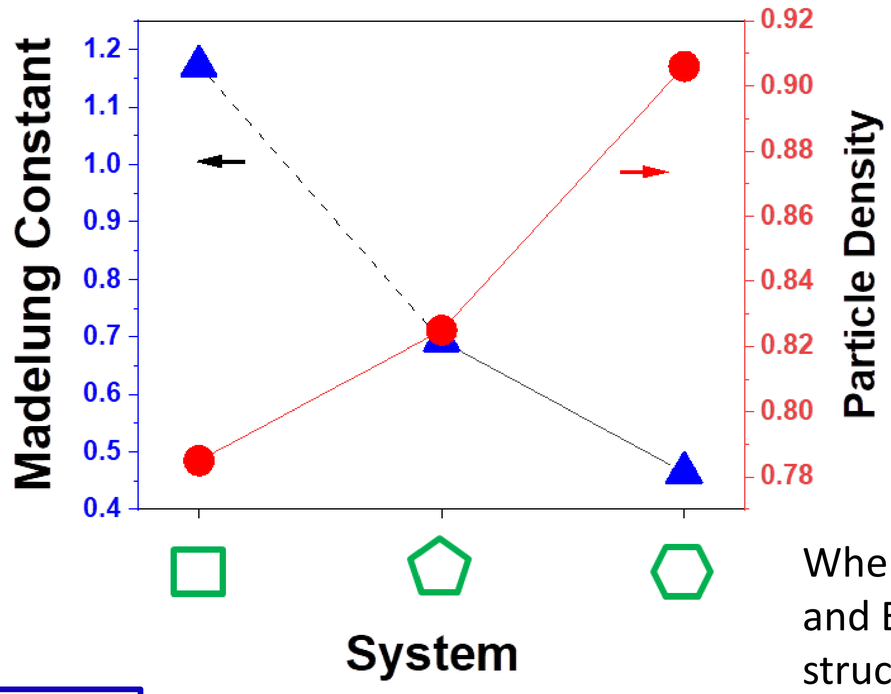
MOTIVATION & INTRODUCTION

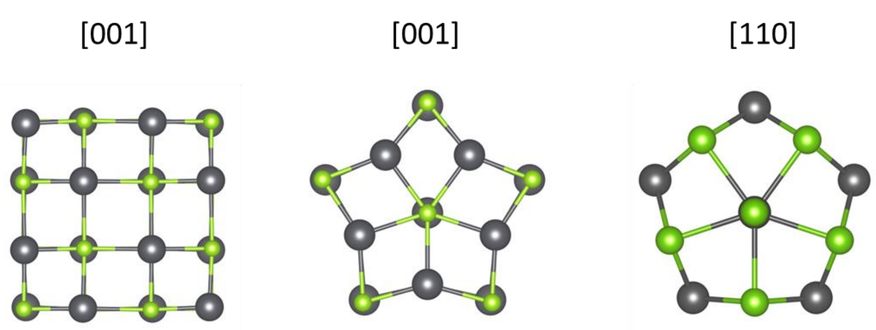




Courtesy: Jakub Polaczyński

Ionic vs Covalent Character





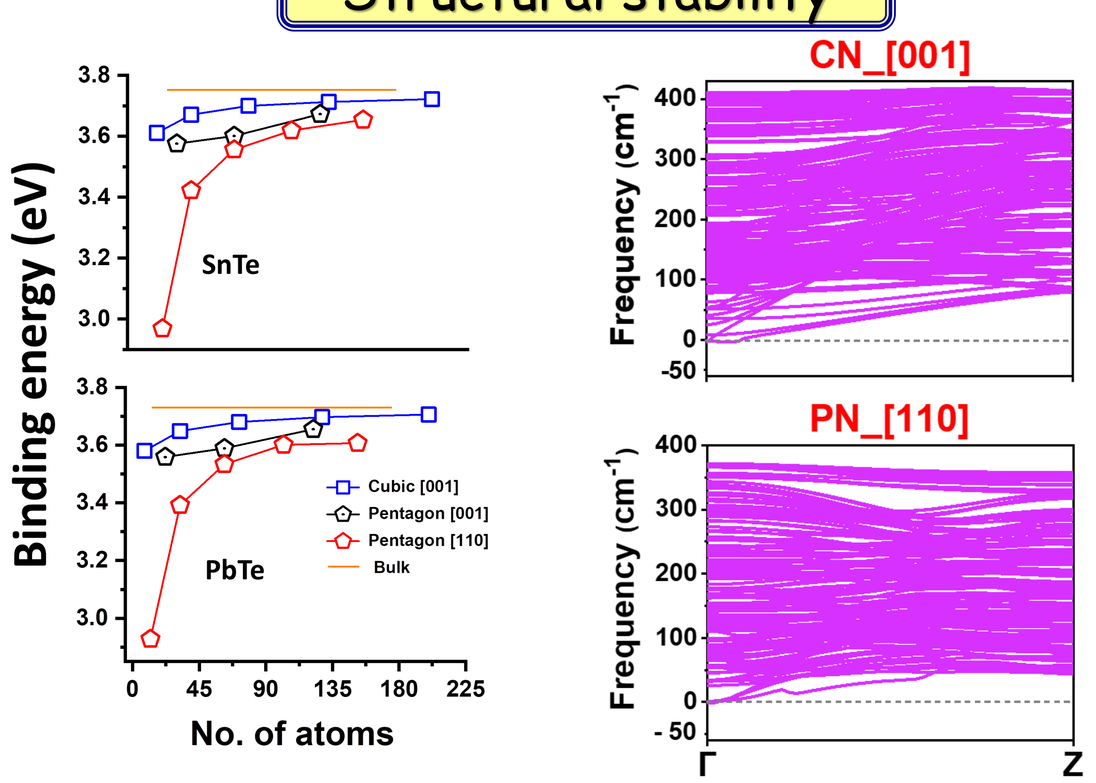
Binding Energy for structural stability

$$E_b = \frac{n_1 E_X + n_2 E_Y - (E_{XY})}{n_1 + n_2}$$

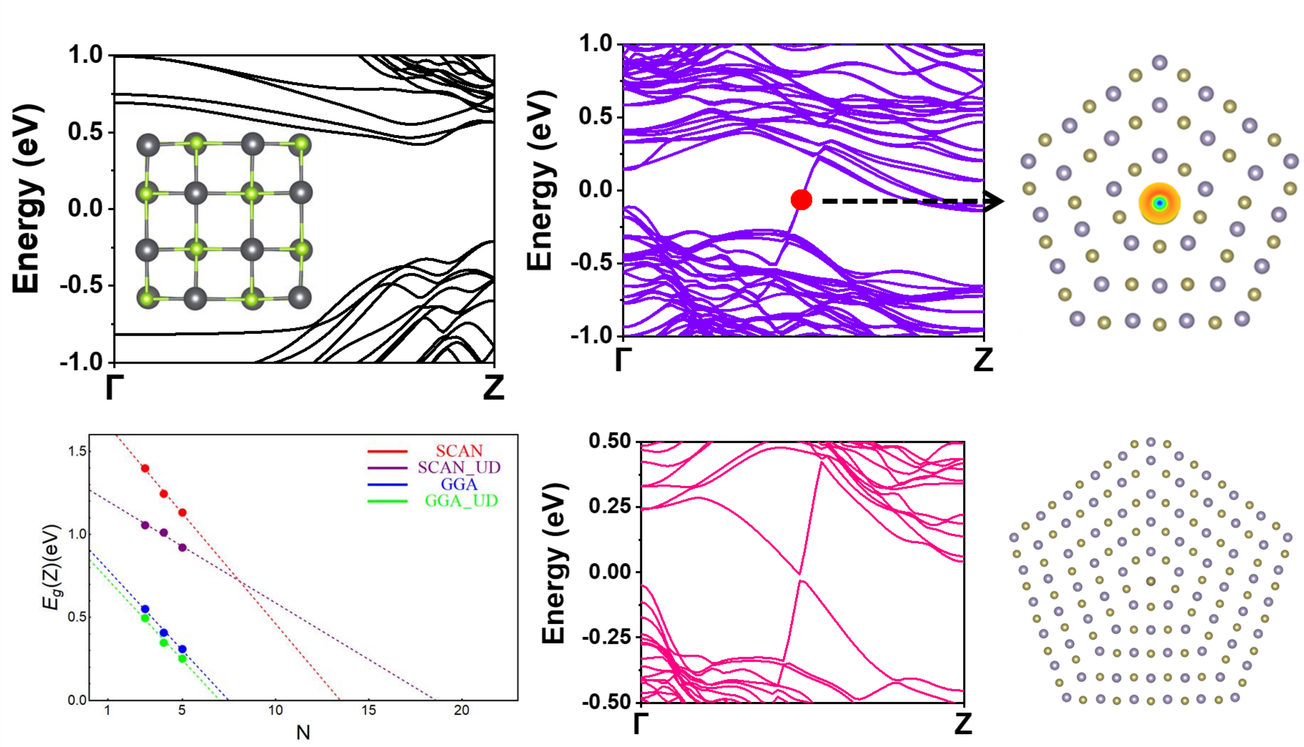
Where n_1 and n_2 are the numbers of X and Y atoms and E_X, E_Y and E_{XY} are the ground state energies of X, Y and optimized structure, respectively.

RESULTS

Structural stability



Electronic properties



CONCLUSIONS

- The pentagonal structure bears intermediate values for Madelung constant and particle density implying that if the bond is partially ionic and partially covalent, pentagonal system is expected to be the most stable one.
- Structural stability increases with the thickness of NWs. Also, both cubic and pentagonal nanowires are dynamically stable.
- Topological transition is estimated in SnTe CNs for thicknesses larger than 13 nm.
- The bands connecting valence and conduction electrons in the trivial PNs originate from the disclination and produce a transition from insulator to metal.