Electronic properties of bare and functionalized 2-Dimensional Tellurene structures

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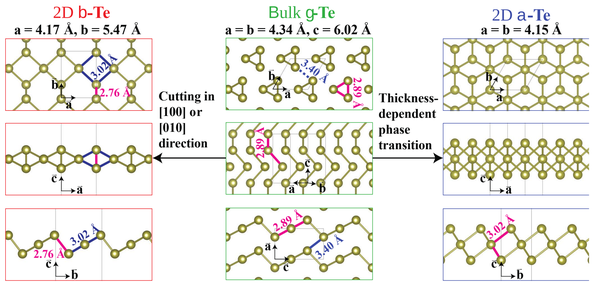
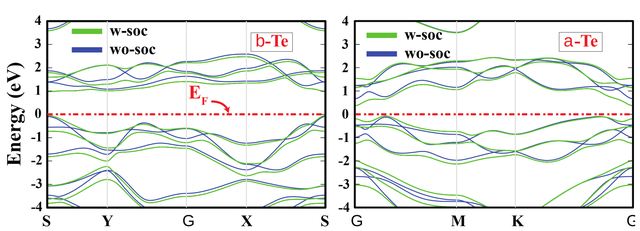
Introduction

- Recently, 2D Tellurene (Te) structures have been experimentally synthesized. These structures possess high mobility and stability which make them ideal candidates for applications in optoelectronics and energy devices.
- We performed density functional theory (DFT) and molecular dynamics (MD) simulations to investigate the stability and electronic structure of 2D α and β-Te sheets, and hydrogen, oxygen, and fluorine functionalized counterparts with various concentrations of adatoms. We also studied the stability of these sheets on Gallium Selenite (GaSe) substrate.
- Our results indicate that Tellurene monolayers, and functionalized counterparts can be synthesized on GaSe and are not only suitable for future optoelectronic devices, but can be used as metallic contacts in nanoscale junctions.

Bare 2D Tellurene

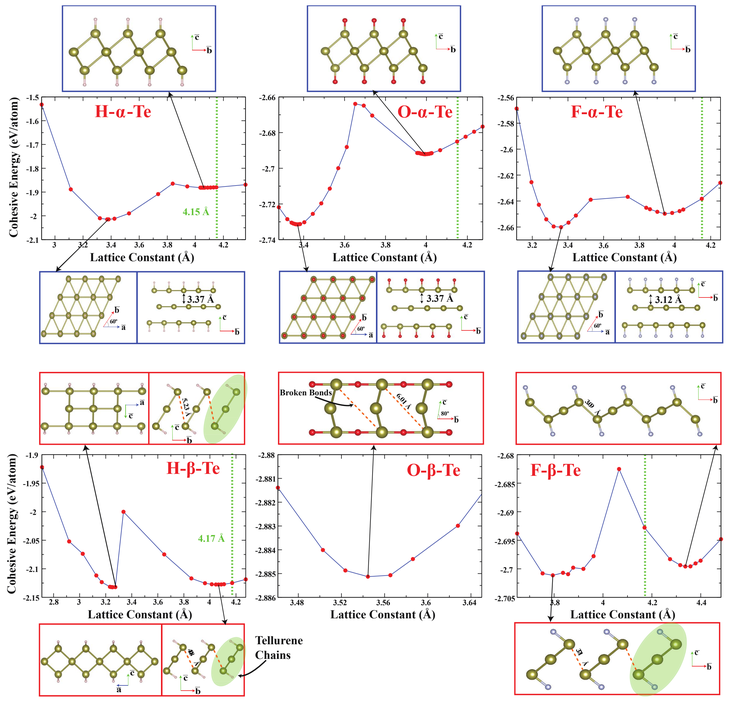


Helical chain structure of ɣ-Te, rectangular structure of β-Te, and hexagonal structure of α-Te.

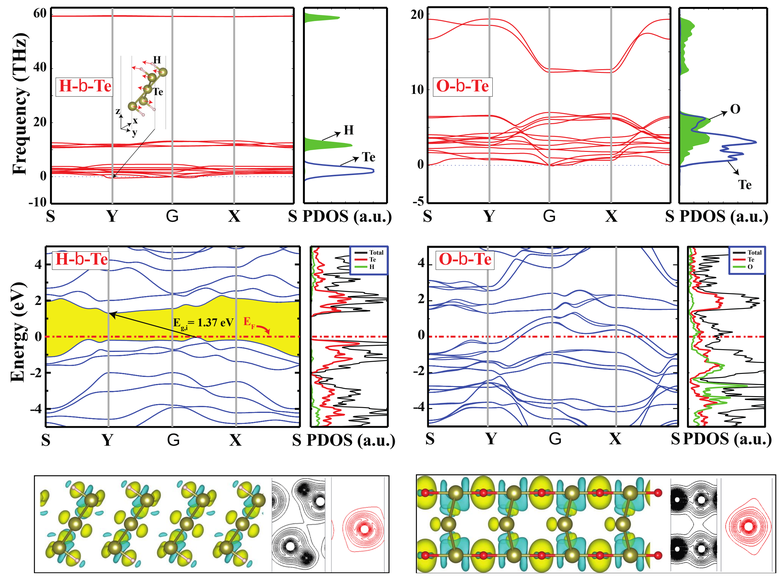


Electronic band structure of bare β-Te with a band gap of 1.02 eV and bare α-Te with a band gap value of 0.56 eV with (green) and without (blue) spin-orbit coupling (SOC) effects.

Functionalized 2D Tellurene

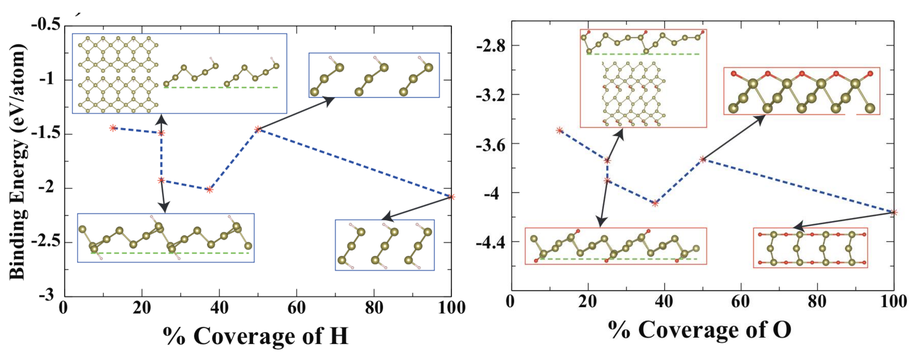


The cohesive energy (in eV/atom) as a function of lattice constant for 2D α and β-Te functionalized with H, O and F. We observe a local and global energy minima for all structures (except O-β-Te).



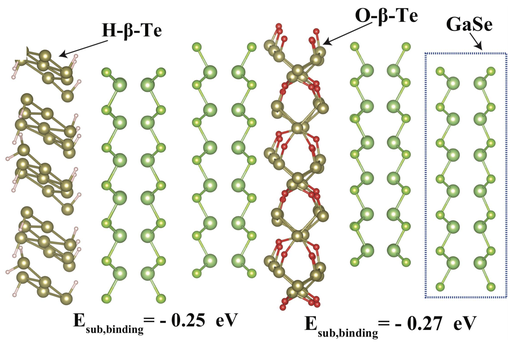
The phonon band structure and phonon projected density of states (PDOS) in addition to the electronic band structure and orbital projected density of states (PDOS) of H-β-Te and O-β-Te. Charge differences with yellow for accumulation and green for depletion.

Adatom Coverage Effects



Binding energy per adatom as a function of H and O coverage on β-Te.

Substrate Effects



Optimized H-β-Te and O-β-Te on GaSe substrate.

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