Band Gaps Engineering inthe 2D $Mo(S_{1-X},Te_X)_2$-Alloy Adsorbed on Graphite, or Sandwiched Between Two Layers of Graphene

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Abstract:
First principles VASP[1] formation-energy calculations were performed for: (1) a $Mo_9(S_{18-m},Te_m)$-2D-alloy (m=0,1,…18) adsorbed (van der Waals bonded[2] to four layers of Graphite (a 4x4x2 155-atom supercell); and (2) a $Mo_8(S_{16-m},Te_m)$-2D-alloy (m=0,1,…16) between two layers of Graphene (an 80 atom supercell). Atomic positions and cell dimensions were fully relaxed, and band gaps (BG) were calculated with a perl script, from VTSTscripts[3].

Band Gaps were calculated for supercells (1) and (2) above, and for the various 2D-alloy (chemical) configurations in vacuum, Figures 1 and 2. All predicted BG are direct. The trends predicted for 2D alloys in vacuum are as one would expect given the difference in electronegativities: S-rich configurations correlate with larger BGs that Te because Shas a larger electronegativity (holds e- more tightly than Te). But when van der Waals bonded to Graphite or Graphene the trend is reversed; evidently, Graphite (Graphene) is an e- source for S and sink for Te.

These results suggest that for BG-engineering materials such as $Mo(S,Se)_2$, $Mo(Se,Te)_2$, and $Mo(S,Te)_2$, using a conductive substrate such as Graphite (Graphene) strongly influences the BG, relative to what is predicted in vacuum.

In addition, aspects of phase stability and phase transitions will be discussed: e.g. in bulk $Mo(Se_{1-X},Te_X)_2$ alloys are predicted to phase separate, whereas, they are predicted to order when they are adsorbed on Sapphire, or Graphite, or sandwiched between Graphene layers.

Keywords: 2D $Mo(S,Te)_2$ alloy; TMD; Band Gaps; First Principles; Graphite; Graphene.

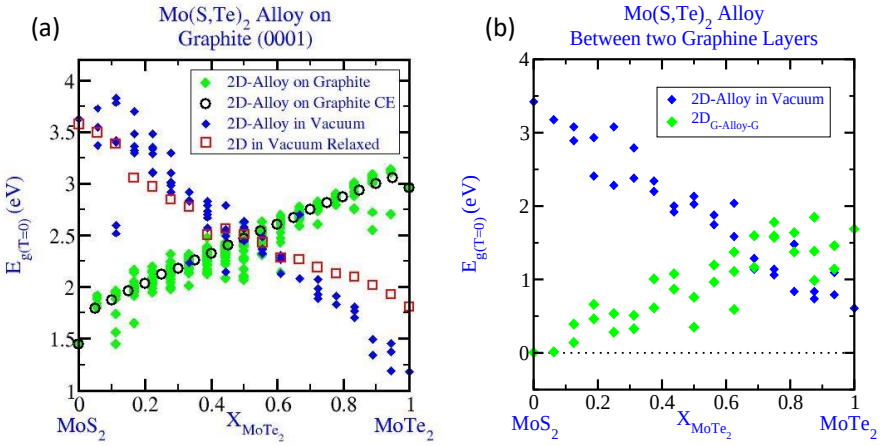

Figure: (a) Calculated band gaps for the $Mo_9(S_{1-X},Te_X)$-2D-alloy adsorbed on Graphite (green), and in vacuum (blue); relaxed in vacuum (red); Black circles (CE) were calculated via cluster expansion; **(b)** Calculated band gaps for the $Mo_9(S_{1-X},Te_X)$-2D-alloy sandwiched between two layers of Graphene (green) and in vacuum (blue).

References:

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