ELECTRONIC STRUCTURE OF THE InSb/CdTe/α-Sn INTERFACE VIA DFT: USING CdTe AS A BARRIER

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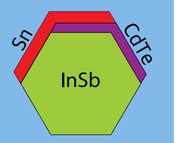
INTRODUCTION

We simulate a tri-layer system composed of InSb, CdTe and α-Sn via DFT. CdTe is proposed as a barrier to mediate the coupling between InSb and α-Sn. These materials are relevant for Majorana zero modes experiments.

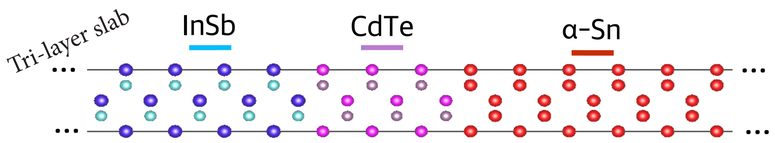
BACKGROUND/ MOTIVATION

- Majorana zero modes (MZM) could be utilized in quantum computing
- They are hypothesized to appear in solid state semiconductor-superconductor hybrid systems
- Experiments use semiconductor nanowires (e.g. InSb) coated with superconducting shells (e.g. Sn)
- Conclusive evidence not yet found so further experimental design and material advancement is required
- Coupling of the semiconductor and superconductor can be too strong leading to "metalization" of semiconductor and unaccessible to Majoranas. Could mediate coupling with a barrier (e.g. CdTe)
- DFT can quicken investigations into the electronic effects of relevant materials and their interfacing for MZM experiments



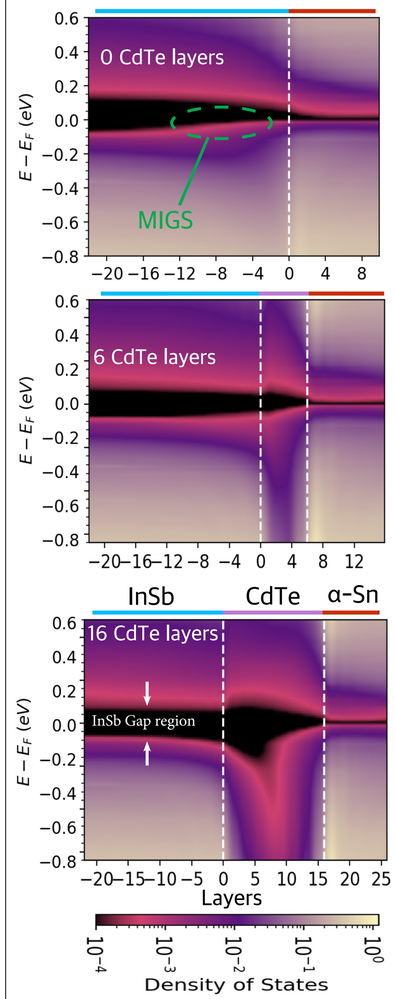
METHODS

Density functional theory (DFT) is a first principles method to conduct electronic structure simulations. The implemented DFT+U approach allows large system simulations at a reasonable computational cost. The U is determined by machine learned Bayesian optimization methods by matching to benchmark HSE band gap and band structure simulations. Slab models are built (shown below) with a varying number of CdTe barrier layers.



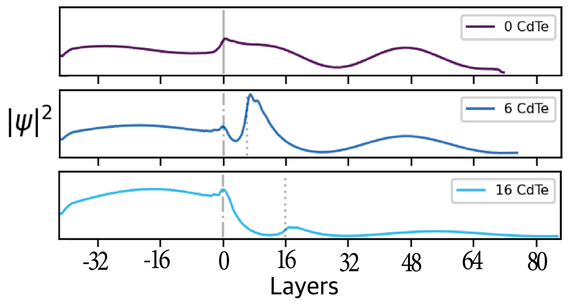
RESULTS

CdTe could offer a barrier to the electronic effects between an InSb/α-Sn interface with a 4 nm interlayer. This could mediate the strength of the coupling and metalization of the interface offering a path to MZM.

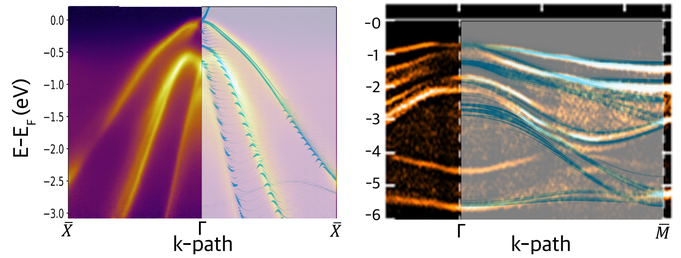


- (Left) The layer by layer density of states (LDOS) for tri-layer slab for different number of CdTe barrier layers is shown.
- With 0 CdTe layers metal induced gap states (MIGS) from the Sn occupy the gap region of the InSb near the interface.
- With 16 CdTe layers we see the normal InSb bulk gap near the interface, suggesting this is an effective tunnel barrier for electronic effects between the InSb and Sn.

(Below) The positional dependence of the electron density associated with the InSb conduction band, for different number of CdTe barrier layers. It obtains more weight in the InSb slab with more CdTe layers due to the exponential decay through the CdTe



EXPERIMENTAL COMPARISON – ARPES



ARPES experimentally maps out the band structures of materials in the Brillouin Zone which can be reproduced in DFT. Comparisons can confirm DFT is producing reliable results while elucidating experimental details of the material. (Left) High energy ARPES of 13 layer thick α-Sn taken at UCSB with 50 layer DFT comparison overlayed. This shows good quality comparisons of the general band structure. (Right) Low energy data of CdTe ARPES data taken by Ren et. al. [1]. The comparisons show that DFT can reproduce low energy features such as surface states.

LIMITATIONS/ FUTURE WORK

- Slab size can lead to quantum confinement effects that give qualitative results on band gap and band structure. However large slabs can make results quantitative.
- No strain in the α-Sn in simulations which is present in experiment
- Only consider electronic effects. Need to infer effect on mediation of metalization with barrier. This could be implemented with Poisson-Schrodinger model
- Next steps to try other materials relevant to MZM experiments, e.g. InAs
- Experimental work of growing these materials has already been done
- Implement barrier fully in experimental set-up

CONCLUSION

- Atomic level simulations of a tri-layer slab composed of InSb, CdTe and α-Sn in DFT were done
- With 3 or 4 nm of CdTe this could provide an barrier to the electronic coupling between InSb and α-Sn.
- Large band gap semiconductors could be useful as a barrier for mediating the superconducting and electronic coupling in Majorana experiments, as well as protecting the device from the environment.

[1] - Ren et. al. Phys. Rev. B 91, 235303