First principles assessment of prospective tunnel barriers at semiconductor/superconductor interfaces

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Majorana zero modes, with prospective applications in topological quantum computing, are expected to arise in semiconductor-superconductor interfaces. However, this interfacing can lead to detrimental effects such as band bending and the loss of necessary semiconductor properties [1]. We study semiconductor-superconductor interfaces relevant to Majorana zero mode systems, introducing barriers to control these detrimental effects, via density functional theory (DFT).

InAs and InSb based devices are popular choices for Majorana zero mode setups due to their large spin orbit coupling and growth properties. Metallic superconductors, such as Al and α-Sn, supply the necessary superconducting effect. To moderate the detrimental effects in the semiconductor from this interfacing, the favorably lattice matched materials of CdTe, ZnTe, and CdSe are explored as tunnel barriers between the semiconductor-metallic superconductor interface.

The PBE+U method is used, with the Hubbard U parameters found via a machine-learned Bayesian optimization algorithm, allowing the simulation of large interfaces. We use the in-house program OGRE[2] to build the reconstructed and relaxed interface models required for these systems.

We then study the band offsets and the penetration depth of metal-induced gap states (MIGS) in bilayer and trilayer interfaces. We first consider the semiconductor-semiconductor, such as InSb/CdTe and InAs/ZnTe, and the semiconductor-metal interfaces, and then move on to the tri-layer interfaces of InSb/CdTe/α-Sn and InAs/ZnTe,CdSe/Al. We study the effect of increasing the thickness of the barrier layers. We find that 16 atomic layers (3.5 nm) of CdTe can serve as a tunnel barrier, effectively shielding the InSb from MIGS from the α-Sn. This, and insights on the InAs-Al interface, may guide the choice of dimensions of the barrier to mediate the coupling in semiconductor-superconductor devices in future Majorana zero modes experiments.

[1] Jardine, M.J. et al. (2023) 'First-principles assessment of CdTe as a tunnel barrier at the α-Sn/InSb interface', ACS Applied Materials & Interfaces, 15(12), pp. 16288–16298. doi:10.1021/acsami.3c00323.

[2] Moayedpour, S. et al. (2021) 'Structure prediction of epitaxial inorganic interfaces by lattice and surface matching with Ogre', The Journal of Chemical Physics, 155(3), p. 034111. doi:10.1063/5.0051343.