Procedural Determination of Novel Stoichiometric Topological Superconductors through Surface and Pressure Effects

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Recently, topological superconductors have attracted great interest as a groundbreaking platform to allow for fault-tolerant quantum computing and overcome the limitations of classical processors defined by Moore’s law. Due to the robust properties of their Majorana fermion surface states, topological superconductors are considered a leading solution to the longstanding challenge of quantum decoherence (i.e. the rapid loss of information to the environment) faced by quantum computers. We proposed eight novel topological superconductors, ABX2 (A=Bi, In; B=Nb, Ta; X=Se, S) and introduced a new systematic methodology to realize topological superconductors by combining transition metal dichalcogenides with spin-orbit post-transitional elements. Utilizing density functional theory, we computationally modeled our materials and determined topological surface states and bulk superconductivity. In addition, we theoretically demonstrated the robust nature of our materials. Based on our simulations under high-pressure conditions, our materials’ non-trivial topology and superconductivity were maintained. These eight compounds are novel due to their bulk superconductivity and intrinsic topological surface states which can be realized without any tampering, a coveted quality for topological superconductors. Using our methods, we replicated the band structures from a publication of an experimentally confirmed topological superconductor, building confidence in our methods selection. Our research holds great promise towards the practical realization of fault-tolerant quantum computers through their ability to eliminate the longstanding problem of quantum decoherence within quantum computational systems.

Awards Won:

National Security Agency Research Directorate : Honorable Mention "Physical Science"