First-Principles Assisted Design of Molecular Scale Graphane Analogues

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Graphene's success has shown that it is not only possible to create stable, single-atom thick sheets of a crystalline material, but that these materials can have electronic properties that are fundamentally different than the parent. Recent work at The Ohio State University has shown that unique single-layer 2D materials based on group-IV elements and especially germanium can be synthesized, stabilized by appropriate ligands [1]. In this talk, we will discuss density-functional theory predictions of structure, properties, defects and transport in such graphane analogues, as well as their experimental realization and validation. Examples discussed include electronic and conduction properties [2] and their strain- [3] and ligand-tunability (Fig. 1) [4,5], as well as point defects and oxidation mechanisms and their experimental observation.

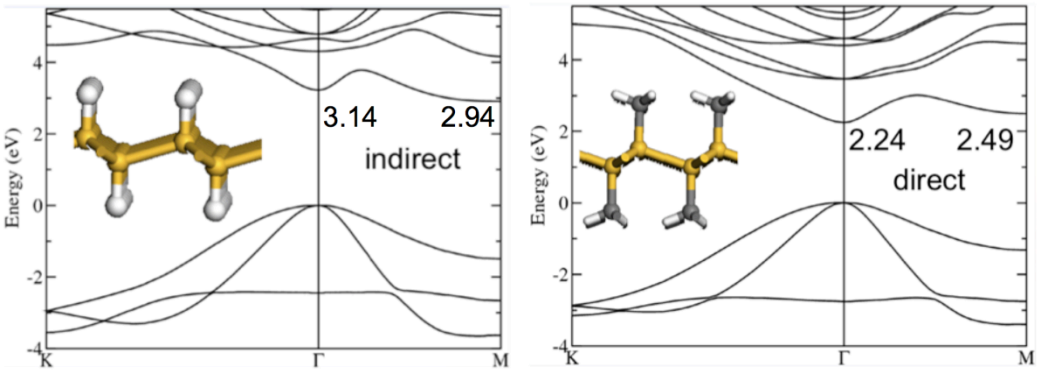

Figure 1 Band structure of silicane with H (left) and CH3 (right) ligands, calculated with HSE06 hybrid potentials [5].

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