Abstract Submitted
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Theory of unsaturated silicon lattices[1] FENG ZHANG, DAVID STUCKE, DRAGAN STOJKOVIC, VINCENT CRESPI — Several molecules are known to contain stable silicon double or triple bonds that are sterically protected by bulky side groups. Through first-principles computation, we demonstrate that well-defined π bonds can also be formed in two prototypical *crystalline* Si structures: Schwarzite Si-168 and dilated diamond. The sp^2-bonded Si-168 is thermodynamically preferred over diamond silicon at a modest negative pressure of -2.5 GPa. Ab-initio molecular dynamics simulations of Si-168 at 1000 K reveal significant thermal stability. Si-168 is metallic in density functional theory, but with distinct π-like and π^*-like valence and conduction band complexes just above and below the Fermi energy. A bandgap buried in the valence band but close to the Fermi level can be accessed via hole doping in semiconducting $Si_{144}B_{24}$. A less-stable crystalline system with a silicon-silicon triple bond is also examined: a rare-gas intercalated open framework on a dilated diamond lattice.

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