Extended sp^3 carbon materials from high pressure

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Abstract

Diamond is the best example of extended, high-pressure sp^3 (tetrahedral) carbon. Other examples are actually rare, despite numerous predictions of low-energy sp^3 allotropes and compounds. In this talk, I will give an overview of two strategies that we are using to close this gap. This first involves manipulating thermodynamics by elemental substitution, which led to the discovery of a new class of sp^3 B–C clathrate compounds with composition MB_3C_3 (M = metal). These compounds have tunable electronic structures and can be semiconductors, metals, superconductors or magnets depending on the metal guest. We demonstrate superconductivity with T_c above 20 K for SrB_3C_3 and predict T_c approaching 100 K at 1 atm for other compositions. The second approach involves high-energy molecular precursors that are strategically arranged to control reactions along specific pathways. In one dimension the products are sp^3 carbon "nanothreads" for which we have determined predictive design rules and can now control with chemical precision.