

First-principles studies of the structural and electronic properties of rigid carbon nanofoam

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Using *ab initio* density functional calculations, we investigate the structural and electronic properties of porous schwarzite structures formed by sp^2 carbon minimal surfaces with negative Gaussian curvature. We calculate the equilibrium geometries, elastic properties and electronic structure of two systems with cubic unit cells containing 152 and 200 carbon atoms, which are metallic and very rigid. The porous schwarzite structure can be efficiently doped by electron donors as well as acceptors, making it a promising candidate for the next generation of alkali ion batteries. Furthermore, the schwarzite structures can be magnetic when doped and thus act as arrays of interconnected quantum spin dots. We also propose that two interpenetrating schwarzite structures be used as a ultimate super-capacitor.