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Designing rigid carbon foams¹ SORA PARK, JEUNG-SUN AHN, YOUNG-KYUN KWON, Kyung Hee University, KRITSADA KITTIMANAPUN, DAVID TOMÁNEK, Michigan State University — We use *ab initio* density functional calculations to study the stability, elastic properties and electronic structure of contiguous sp^2 carbon networks with negative Gaussian curvature, called schwarzites. We find these structures, which may be thought of as dense arrays of inter-connected nanotubes, unusually rigid. We focus on two systems with cubic unit cells containing between 152 and 200 carbon atoms, which we find metallic. The contiguous internal graphitic surface of schwarzites subdivides space into two distinct subspaces. Due to the ease of atomic diffusion, schwarzites appear as a useful alternative to graphite electrodes for a new generation of Li-ion batteries. Since the concentration of electron donors or acceptors can be modified reversibly, the doping level of the schwarzite may be tuned in order to optimize specific reactions, including H₂ storage, in the other subspace. The other subspace can alternatively accommodate a duplicate schwarzite structure. The two interpenetrating, but separated structures can be used as electrodes of the ultimate super-capacitor.

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