

Abstract Submitted  
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*Ab initio* studies of defects in carbon nanofoam structures<sup>1</sup> DAVID TOMANEK, ZHEN ZHU, Michigan State University, ARKADY KRASHENINNIKOV, University of Helsinki — We combine *ab initio* density functional and GW calculations to study the stability, electronic and elastic properties of hypothetical cellular foam-like carbon nanostructures. These systems with a mixed  $sp^2/sp^3$  bonding character are structurally related to bundles of carbon nanotubes. The cross-sectional honeycomb structure may accommodate the same type of structural defects as the honeycomb lattice of graphene. The infinite 3D foam structure is a narrow-gap semiconductor, with the binding energy of atoms nearly 0.5 eV lower than graphene. Quasi-2D layered foam structures of finite thickness may be stabilized by terminating caps. When exposed to hydrostatic pressure, the unit cells of the foam deform significantly from their initially hexagonal shape.

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