Abstract Submitted
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Local curvature and relative stability of graphitic carbon nanostructures[1] JIE GUAN, ZHONGQI JIN, DAVID TOMANEK, Michigan State University — We propose a way to estimate the relative stability of graphitic nanostructures including fullerenes, nanotubes and schwarzites using continuum elasticity theory. The key quantity is the local deformation energy with respect to graphene, which we determine by estimating the two principal radii of curvature at each lattice site using the Bertrand-Diquet-Puiseux theorem. We find an impressive level of agreement between strain energies based on local curvature and *ab initio* density functional calculations. We demonstrate that our approach correctly determines strain energy differences between nanotubes with different chiral indices (n,m) and zero Gaussian curvature, C_n fullerenes with $20 \leq n \leq 72$ atoms and positive Gaussian curvature, and selected schwarzites with negative Gaussian curvature. In contrast to other methods, our approach correctly determines even the energy differences between different isomers of fullerenes such as C_{28}, C_{36} and C_{38}.

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