

Relative Stability and Local Curvature Analysis in Carbon Nanotori

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We introduce a concise formalism to characterize nanometer-sized tori based on carbon nanotubes and to determine their stability by combining ab initio density functional calculations with a continuum elasticity theory approach that requires only shape information. We find that the high strain energy in nanotori containing only hexagonal rings is significantly reduced in nanotori containing also other polygons. Our approach allows to determine local curvature and link it to local strain energy, which is correlated with local stability and chemical reactivity.