DFT properties of Quasi-One-Dimensional Nanostructured Materials

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Over the past several years we have made substantial progress in developing an approach for density-functional electronic structure calculations on quasi-one-dimensional nanostructures with helical symmetry. In this talk we discuss the application of these first-principles methods using Gaussian basis sets for calculating the electronic band structure of periodic graphitic nanostructures such as carbon nanotubes and graphene nanoribbons. In particular, we discuss the numerical methods needed to evaluate gradients of the total energy. The gradients with respect to changes in nuclear coordinates have similar algorithms for forces calculated in molecular DFT codes, but the derivatives with respect to changes in lattice spacing and twist are more complex. We present results for the application of these methods to graphitic strips and inorganic nanowires.

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