TAO-DFT and Its Applications to Carbon Nanomaterials

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I will briefly describe thermally-assisted-occupation density functional theory (TAO-DFT) [1], the density functional approximations to TAO-DFT (TAO-DFAs) [2], the hybrid TAO-DFT schemes (i.e., the inclusion of exact exchange in TAO-DFT) [3], and the applications of TAO-DFT to carbon nanomaterials (e.g., acenes, zigzag graphene nanoribbons, cyclacenes, PAHs, linear carbon chains, etc.) [4–8]. In contrast to Kohn-Sham density functional theory (KS-DFT), TAO-DFT is a density functional theory with fractional orbital occupations given by the Fermi-Dirac distribution (controlled by a fictitious temperature), for the study of large ground-state systems with strong static correlation effects. Due to its computational efficiency, TAO-DFT has been recently applied to the study of various carbon nanomaterials with strong static correlation effects (which are challenging systems for conventional electronic structure methods). Some interesting results will be presented in this talk.

References:

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