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**TDDFT excitations in polymer density-functional first-principles calculations** JOHN MINTMIRE, Oklahoma State University — 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 periodic symmetry. This approach calculates a first-principles total energy and band structure using an all-electron Gaussian-basis set. In this talk we discuss the application of a Casida-equation scheme to calculate excitation energies and excited states in such nanostructures within a time-dependent density-functional theory (TDDFT) approach. We present some preliminary results for carbon nanotubes and graphitic nanoribbons where we examine localization trends in the excited states. This research was supported in part by an appointment to the Higher Education Research Experience for Faculty sabbatical program at Oak Ridge National Laboratory program.

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