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Time-Dependent Density-Functional Calculations of Photoabsorption Spectra of Carbon Nanostructures TOMOYUKI NOGUCHI, Tokyo University of Science, CREST, Japan Science and Technology Agency, MASAAKI ARAIDAI, Tokyo University of Science, CREST, Japan Science and Technology Agency, KAZUYUKI WATANABE, Tokyo University of Science, CREST, Japan Science and Technology Agency — Optical properties of nanoscale structures have attracted much attention experimentally and theoretically. It is not appropriate to apply the conventional density-functional theory (DFT) to investigation of the optical properties, because the excited states, which are not adequately represented by the DFT, play essential roles in these phenomena. To go beyond the DFT, we adopt time-dependent DFT (TDDFT) calculations with the linear- response theory, which is a powerful computational tool for calculating the excited states of nanostructures properly. In this study, we report the results of excitation energies and photo-absorption spectra in aromatic molecules, such as naphthalene and anthracene. A high spectral intensity in a low frequency region occurs in the spectra for these molecules. This characteristic spectrum is shifted to lower energy with increasing molecular size. We also discuss the details of the electronic excitations utilizing the TDDFT calculations in a real-time scheme.

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