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Exciton Scattering in Branched Conjugated Molecules: Towards Photoinduced Dynamics and Energy Transfer

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The exciton scattering (ES) approach attributes excited electronic states in quasi-one-dimensional (branched) conjugated molecules with perfect geometry to standing waves on the linear segments of a molecule formed by scattering of quantum quasi-particles (excitons). We extract their dispersion and frequency-dependent scattering matrices at termini, including donor/acceptor substitutions, joints, and branching centers from time-dependent density functional theory (TD-DFT) calculations, with applications to for conjugated phenylacetylene-based molecules. This allows electronic spectra for any structure of arbitrary size within the considered molecular family to be obtained with insignificant numerical effort. To extend the capability of the ES approach to treating photoinduced dynamics, including absorption and fluorescence lineshapes and energy transfer, the methodology should be modified to account for non-ideal molecular geometry. Geometry distortions break down translational symmetry of the linear segments, and excitations are not represented by perfect standing waves anymore. To overcome this difficulty we associate electronic excitations with the eigenstate of a quantum particle on an irregular lattice (graph), referred to as a tight-binding model. The morphology of the underlying lattice, together with the tight-binding parameters, can be identified by studying the topological and analytical properties of excitons at molecular termini, joints, and branching centers. The dependence of the tight-binding parameters on geometry distortions that controls effects of disorder and coupling to vibrational modes can be extracted from quantum chemical calculations by studying exciton scattering on localized geometry distortions, the latter considered as scattering centers.