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Electron transport dynamics of molecular devices: A time-dependent density functional theoretical study in momentum space[1]
ZHONGYUAN ZHOU, SHIH-I CHU, Department of Chemistry, University of Kansas, Lawrence, KS 66045 — We propose a first-principles time-dependent density functional theoretical (TDDFT) approach in momentum (P) space for the quantitative study of electron transport dynamics in molecular devices. This approach is free of self-energy function and memory term and beyond the wide-band limit (WBL). It is computationally considerably more efficient than the conventional TDDFT approach in spatial coordinate (R) space. In this approach, the basic equation of motion is a time-dependent integro-differential equation obtained by Fourier transform of the R-space time-dependent Kohn-Sham (TDKS) equation. It is formally exact and includes all the effects and information of the electron transport in the molecular devices. The electron wavefunction is calculated by solving this equation in a finite P-space volume. This approach has been used to calculate the currents through several one-dimensional systems. The results are in very good agreement with those obtained from other theoretical methods, demonstrating the efficiency and power of this approach.

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