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Time-dependent density-functional theory for real-time electronic dynamics on material surfaces RULIN WANG, DONG HOU, XIAO ZHENG, Univ of Sci & Tech of China — The real-time electronic dynamics on material surfaces is critically important to a variety of applications. However, numerical simulations are rather challenging for conventional first-principles methods such as the time-dependent density-functional theory (TDDFT). To solve this problem, we extend the applicability of TDDFT to open electronic systems[Phys. Rev. B **75**, 195127 (2007)]. The dissipative system-environment interactions are treated by a hierarchical equations of motion (HEOM) approach. The combined TDDFT–HEOM method, along with a k-sampling scheme [J. Chem. Phys. **132**, 114703 (2010)] for calculating the spectral function of a two-dimensional system, is applied to simulate real-time electronic dynamics on material surfaces. Two prototypical scenarios are exemplified [Phys. Rev. B (accepted) (2013)]: the relaxation of an excess electron on a graphene surface, and the electron transfer across the molecule-graphene interface. These two examples accentuate the fundamental importance and usefulness of an open-system TDDFT approach, and they also provide some insights into the characteristic features of temporal electron evolution and dissipation on surfaces of bulk materials.

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