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Dependence of Non-adiabatic Couplings, Energy Levels, and Lattice Ion Movements on Exchange-Correlation Approximations LESHENG LI, JIAN CHENG WONG, YOSUKE KANAI, Univ of NC - Chapel Hill, KANAI GROUP TEAM — Dependence on nonadiabatic couplings (NACs), single-particle energy levels, and lattice ion movements on approximated exchange-correlation (XC) functional is examined for modeling excited electron dynamics using fewest switches surface hopping simulations approach. A representative interface between boron nitride and Li ion was considered because of its strong charge transfer character, and wave function localization can be quite sensitive to the approximated XC potential. Generalized gradient approximation (PBE) and its hybrid (PBE0) are considered in this work. We investigate the extent to which the excited electron dynamics is influenced by XC approximation and how, through examining NAC, energy levels, and lattice ion movements.

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