Full *ab initio* calculations of non-adiabatic electron-atom coupled dynamics

Dongbin Shin, Noejung Park[*]

Department of Physics and Center for Multidimensional Carbon Materials,
Ulsan National Institute of Science and Technology, Ulsan, 689-798 Korea
noejung@unist.ac.kr

Since the Schrodinger's and Dirac's formulation of quantum mechanics at the beginning 20th century, diverse branches of theories have developed to deal with quantum mechanics of condensed matters in a way of as ab-initio as possible. The most widely used method is the density functional theory in which the one body Hamiltonian is solved self-consistently, and atomic degrees of freedoms are singled out through the Born-Oppenheimer approximation. Various hierarchical and complementary treatments have been introduced to overcome limitations of such an effective one-body theory. Now the community in this field is ready to include perturbations, such as photons or electrons colliding with condensed matters, to study sub-femto second phenomena beyond Born-Oppenheimer approximation. As a practical implementation in this direction, we developed the package of real-time time-dependent density functional theory, in which the Kohn-Sham orbitals evolve along with the self-consistent evolution of density and Hamiltonian. We present our results for electron tunneling across an oxide insulator and collision of an electron wave packet in a material system. We particularly put emphasis on the fact that, because of the over-delocalization error of the conventional local density functionals, an explicit control parameter for the electrons correlation, such as Hubbard U term, is necessary in the time-dependent equation. We show that the non-local Hubbard potential can be implemented in, line with other non-local components, in the Suzuki-Trotter's splitting scheme as well as in Crank-Nicolson form of propagator. As example studies, we calculated the high speed motion of alkali atoms on metal surface and the exchange of electron between localized defects and metallic bath, as sketched in the Anderson model.