Modeling Excited Electron Dynamics at Semiconductor-Molecule Interfaces

Scientific Achievement

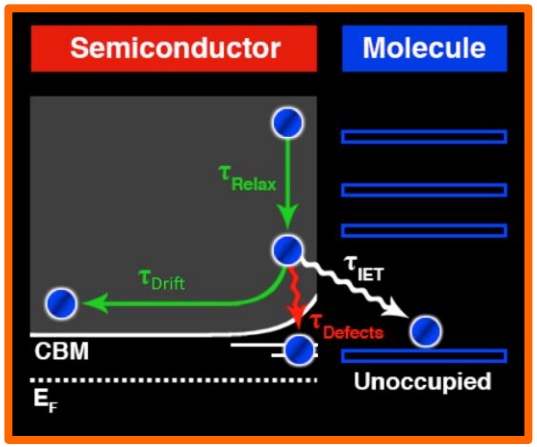
First-principles quantum dynamics simulation approach was developed to model excited electron dynamics at semiconductor-molecule interfaces.

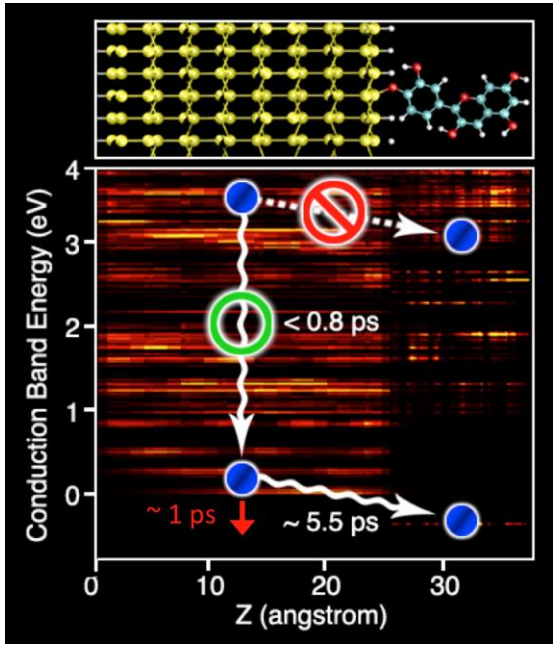
Significance and Impact

The computational approach will help develop a predictive understanding of back electron transfer kinetics, which is governed by several competing mechanisms. Simulation enables us to study how atomistic features (e.g. defects and adsorption sites) influence the complex dynamics.

Research Details

- Many-body perturbation theory, first-principles molecular dynamics, and surface hopping algorithms are combined to model the excited electron dynamics from first principles.
- Interfacial electron transfer was found to take place, following the hot electron relaxation in a representative Type-II heterojunction.
- Hot electron transfer is hardly observed.
- Hot electron can be trapped in a defect state (from surface dangling-bond) quite rapidly.





Lesheng Li and Yosuke Kanai, in preparation.
Work was performed at University of North Carolina at Chapel Hill