

## AB INITIO QUANTUM DYNAMICS ON NANOSCALE

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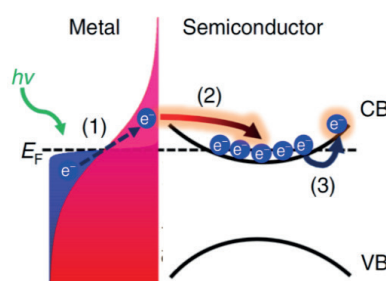
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Excited state dynamics play key roles in condensed phase and molecular materials designed for solar energy, opto-electronics and other applications. To control and steer such far-from-equilibrium processes one has to understand the material's response on nanometer scale and with fine time resolution. We developed approaches for nonadiabatic molecular dynamics and coupled them in a unique way with time-dependent density functional theory to model such non-equilibrium responses at the atomistic level in a broad range of systems.

FRIDAY,  
23.04.2021

2:00 PM

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FURTHER INFORMATION



$$i\hbar \frac{\partial \varphi_p(x,t)}{\partial t} = H\varphi_p(x,t)$$

