Combined light and force-field based molecular dynamics simulation

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We have aimed to develop a novel computational scheme of unified light and molecular dynamics to enable us to describe light-matter interaction in atomistic scale in time-domain by directly incorporating light electric field or electromagnetic field into force-field based molecular simulation (MD). In this talk, we present two methods: (1) Maxwell + polarizable MD multi-scale simulation, and (2) classical electronic and molecular dynamics (CEMD) simulation. The former provides coupled dynamics of electromagnetic wave (Maxwell equation) and molecules in crystalline solid (classical MD) utilizing electronic polarizable force-field model. We perform simulations of vibrational IR and Raman spectroscopies and show their measurement processes in the experimental setup together with motions of propagating light wave signal and molecules. The latter one is capable of describing optical response of metal material under visible light electric field by incorporating classical equation of motion for free electrons on metal in the framework of the force-field model. We show numerical examples of (i) classical image potential, (ii) dielectric function, (iii) absorption spectra and (iv) plasmon resonant excitation and thermal relaxation.