**TDDFT Modeling of Electron-Enhanced Atomic Layer Deposition**

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Electron-enhanced atomic layer deposition (EE-ALD) is the technique required for low thermal budget fabrication of semiconductor devices. From experimental side, it is difficult to provide comprehensive information for revealing specific reaction processes in-depth. To approach this challenge, Time dependent density functional theory (TDDFT) has been proved to be a powerful tool for modeling excited states reactions in EE-ALD. Our theoretical investigations aim at understanding underlying physical mechanisms of the critical reactions controlling the growth rate in, During the EE-ALD reaction process, the energetic incident electrons excite the electronic states of target molecules and stimulate ligand dissociation. From the perspective of theoretical study, the electron-induced dissociation can be separated into two problems: the electron excitation in target molecule by incident electron inelastic scattering and coupled electron-ion dynamics for target molecule in excited state. we systematically calculated ligand dissociation driven by the forced excitation, which demonstrated that single-electron excitation (e.g. HOMO to LUMO) hardly stimulates ligand dissociation. Furthermore, we implemented the incident electron wave packet in TDDFT modeling with plane wave basis code, and calculated the excited state dynamics process for incident electron scattering on target molecule – Co ALD precursor Co(CO)3NO. Our results show that when colliding by the incident electron wave packet with kinetic energy of 50 eV, the ligand dissociation hasn’t happened in precursor molecule.