Physics & Astrophysics Colloquium

Light-to-Matter Interaction

Physicist' vs. Chemist' Point of View

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4:00 PM Friday, February 24, 2023, Room 211, Witmer Hall

Abstract:

Interaction of matter to electromagnetic field can be considered as a center of applied science. Characterization and probing, in broad spectral ranges from NMR to X-ray, as well as promoting a sample into an excited state deals with interaction of matter to electromagnetic field. Two examples of such interaction are of key interest for molecular systems: IR resonant excitation of molecular vibrations and UV-vis excitation that allows molecular system to explore excited state potential energy surface. Both types of pulse of continuous excitations are capable to drive molecular system away from the equilibrium and facilitate bond breaking events, i.e. photochemistry. Pulse and continuous excitations represent a paradigm of external electromagnetic radiation. Since recently, the research community realizes an importance of electromagnetic radiation of microcavities. The electromagnetic radiation of a resonant cavity gives and takes energy to/from molecular system placed in the center of cavity, even in the absence of external excitation. A mode of a cavity and electronic or vibrational state of the molecular system are coupled, and form a bound matter to field state, often referred to as a "polariton". This talk covers several algorithms for treating matter-to electromagnetic radiation interaction at different level of approximations: (i) bound state, (ii) external continuous excitation, and (iii) short time pulse excitation in the IR and UV-vis ranges. All algorithms use on-the-fly *ab initio* molecular dynamics and electronic structure for parameters. The algorithms are illustrated by applications to several models. Vibrational polariton algorithm is applied to explore hydrogen fluoride molecule in the IR cavity. Time-dependent excited state dynamics (TDESMD) algorithm is applied to photoactivated formation of luminescent defects at surface of carbon nanotubes. An implementation of Redfield approach for instantaneously excited electronic state is applied for exploring photoluminescence of silicon carbide nanoparticles in presence of surface defects.

Refreshments at 3:30 PM in Witmer Hall, Room 215

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