GESELLSCHAFT DEUTSCHER CHEMIKER

ORTSVERBAND HANNOVER

Einladung zum GDCh-Colloquium des Ortsverbandes Hannover

Das Colloquium findet um 17h c.t. im Dr.-Oetker-HS (Raum 007, Gebäude 2504) der Leibniz Universität Hannover, Institut für Physikalische Chemie und Elektrochemie, Callinstraße 3a, D-30167 Hannover statt.

19.12.2024 **Prof. Dr. Robin Grotjahn**
Santa Clara University, CA

Tackling Major Challenges for Time-Dependent DFT:
Triplet States, Charge-Transfer Excitations, and Gauge Variance

Due to its excellent cost-performance ratio, time-dependent density functional theory (TDDFT) in its linear-response implementation is often the method of choice for studying the photophysical and photochemical properties of large molecules. Here it is shown how the practical limitations of TDDFT for the study of triplet and charge transfer states are overcome by the new classes of local hybrid and range-separated local hybrid functionals. Investigations of singlet fission chromophores, phosphorescent emitters, and carbene species demonstrate the robustness and efficiency of these methods as practical tools.

On a much more fundamental note, spurious TDDFT errors, sometimes exceeding 0.5 eV, with meta-GGA exchange correlation functionals are analyzed. It is demonstrated that this problem is rooted in the gauge dependence of the implementation of these functionals in most contemporary quantum chemical software packages. It is shown how the problem can be completely eliminated by the inclusion of the paramagnetic current density. Recent extensions of this formalism to excited state properties and quadratic response theory ensure reliable predictions of excited state structures and two-photon absorption spectra.

Prof. Dr. Jens-Uwe Grabow
Vorsitz OV Hannover

Vor dem Colloquium findet ab ca. 16h c.t. eine ‚Kaffeerunde' mit dem Vortragenden in der Bibliothek des PCI statt.