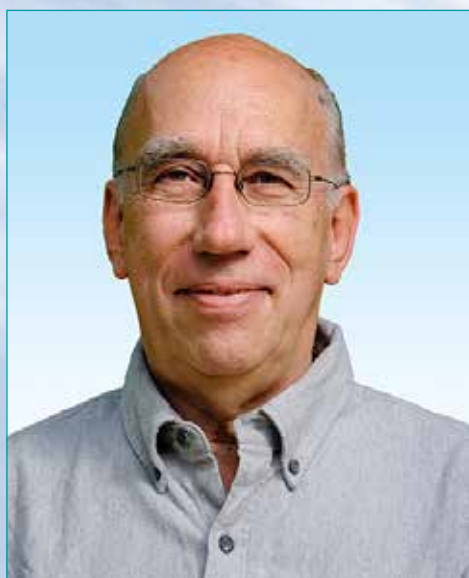


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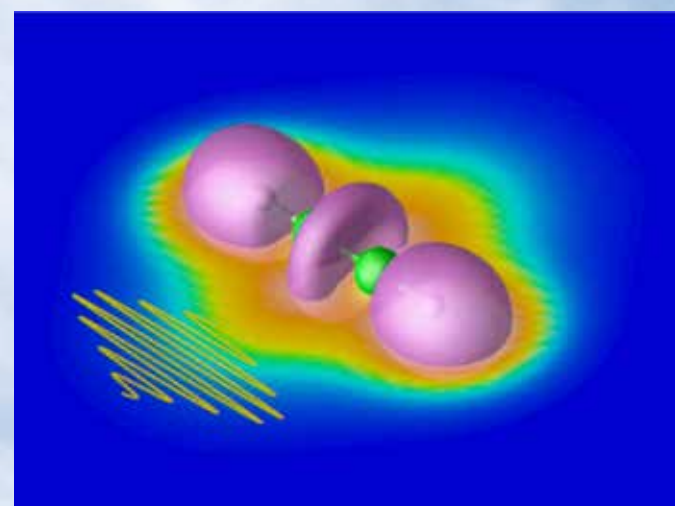
ELECTRONS DANCING TO THE RHYTHM OF LIGHT: INSIGHTS FROM TIME-DEPENDENT DENSITY-FUNCTIONAL SIMULATIONS



by Eberhard K.U. Gross

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This lecture is about the dynamics of electrons, how it can be monitored, analyzed and, ultimately, controlled on the femto-second time scale. Time-dependent density functional theory (TDDFT) will be presented as a versatile theoretical method to describe the dynamics of electronic systems from first principles. While early applications of the method focused on the response to weak probes, real-time TDDFT simulations of strongly driven systems have recently enjoyed increasing popularity in predicting the dynamical behavior far from thermal equilibrium. We shall visualize the laser-induced formation and breaking of chemical bonds, and we shall highlight non-steady-state features of the electronic current through nano-scale junctions. Under certain conditions, these currents can induce forces on the nuclei that trigger a trapped molecule to rotate, thus leading to an electronic “waterwheel”. Furthermore, with the goal of pushing magnetic storage processes towards ever shorter time scales, we demonstrate that, with ultrafast laser pulses, the local magnetic moment of a sub-lattice of the material can be transferred to another sub-lattice within a femto-second or faster. This optically induced spin transfer is a million times faster than the read-write process in present-day magnetic storage devices.



Visualizing the electron localization in acetylene.

THURSDAY
FEBRUARY
26, 2026

5 pm - 6:15 pm
LECTURE HALL
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