ID: Plenary I

Title: Physics on the Femto-Second Time Scale: Analysis and Control of Electronic Motion

Name: Gross, E. K. U.

Affiliation: Max Planck Institute of Microsrtructure Physics

Time-dependent density functional theory (TDDFT) has become the method of choice to calculate the optical spectra of large molecules. After an overview of the basic concepts of TDDFT and some recent advances in the calculation of excitonic spectra for bulk insulators [1], TDDFT will be employed to visualize, analyse and, ultimately, control electronic motion on the femto-second time scale. Three recent developments beyond the linear-response regime will be presented: (i) The time-dependent electron localization function (ELF). This quantity is derived from the conditional probability of finding an electron in the vicinity of a point r if one knows with certainty that there is another electron with the same spin at r. The shape of the ELF (as function of r) provides a topological classification of the different types of chemical bonds. In the time-dependent case, the ELF allows one to visualize the formation and breaking of chemical bonds in a laser field in real time [2]. The sequence of snapshots below shows a laser-induced p-p* transition in acetylene. Questions like: ?How much time needs an electron to complete a transition from one state to another? ? can be addressed in this way.