CFEL SCIENCE SEMINAR

July 23rd, 2010, 10.00 a.m. – DESY Bldg. 49, Room 108

Sang-Kil Son

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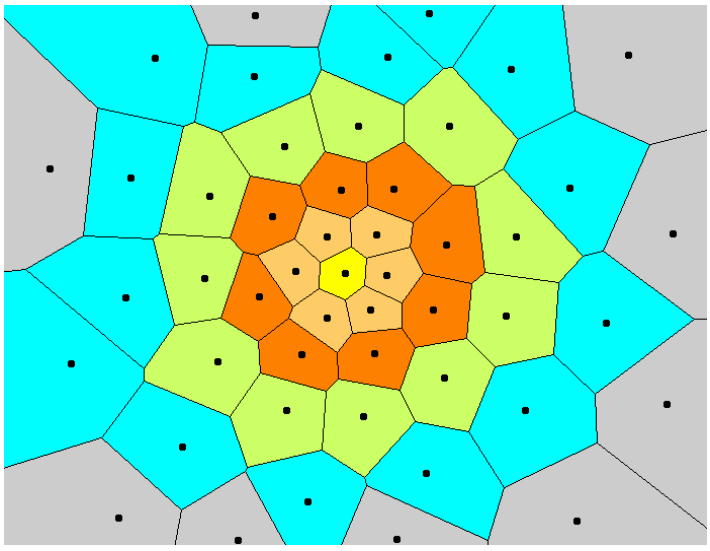
Theoretical study of strong-field multiphoton ionization of polyatomic molecules: a new time-dependent Voronoi-cell finite difference method

We present time-dependent density-functional theory (TDDFT) studies of multiphoton ionization (MPI) of several polyatomic molecules in intense short-pulse laser fields with proper treatment of multielectron effects.

For an accurate all-electron solution for polyatomic molecules, we develop a new time-dependent Voronoi-cell finite difference (TDVFD) method with highly adaptive multicenter molecular grids.

We apply the method to investigate the orientation dependence of MPI of N_2, CO_2, and H_2O, revealing the importance of multielectron effects from multiple orbital dynamics.



Host: Robin Santra, CFEL Theory Group