Max-Planck-Institut für Struktur und Dynamik der Materie

Max Planck Institute for the Structure and Dynamics of Matter

Friday, November 4th 2016 - 10:00
CFEL Seminar room IV (Bldg. 99)

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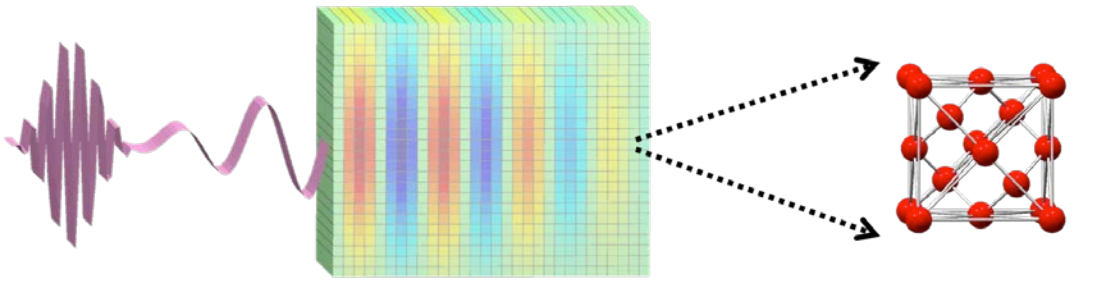
TDDFT in solids for electron dynamics induced by ultrashort laser pulses

Since 2000, we have been developing a real-time, real-space computational method based on time-dependent density functional theory to describe electron dynamics in crystalline solids induced by light pulses. In a microscopic scale, we solve the time-dependent Kohn-Sham equation in a unit cell of solid treating the applied electric field is by the vector potential. We further combine the microscopic calculation with the dynamics of light electromagnetic field in a multiscale modeling, as describe in the figure. In my presentation, I first explain our method including some historical aspects. Then I will show some recent and on-going applications such as energy transfer from a femtosecond laser pulse to electrons in quartz and graphite, and ultrafast changes of dielectric properties of diamond by an intense laser pulse.



Macroscopic system
(Electromagnetics)

$$\left(\nabla^2 - c^{-2}\partial_t^2\right)\mathbf{A} = -4\pi\mathbf{J}/c$$

Microscopic system
(Quantum mechanics)

$$i\hbar\partial_t\Psi = \hat{\mathcal{H}}\Psi$$

Host: Angel Rubio

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