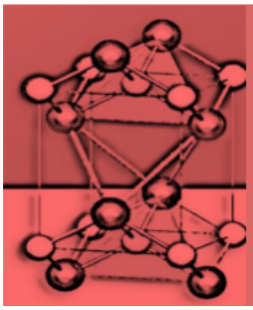

IX Workshop on Novel Methods for Electronic Structure Calculations

10th – 19th November 2021
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Simulation of electron dynamics with real-time TDDFT: Application to electronic stopping

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In this talk I will briefly review ground state DFT and its use in ab initio molecular dynamics simulations, comparing Born-Oppenheimer (BOMD) and Car-Parrinello (CPMD) approaches. Then I will introduce time-dependent DFT (TDDFT) to describe electronic excitations and will discuss its properties, advantages, and limitations as well as similarities and differences with CPMD. I will then focus on the use of TDDFT in its real-time version for the simulation of electronic stopping in materials, showing results for a variety of systems that span from crystalline solids to disordered molecular systems. I will pay special attention to the case of water, which is frequently used as a model medium to describe the irradiation of biological systems. I will also show some recent results of the irradiation of DNA in the presence and absence of the aqueous medium. I will use the example of water to illustrate statistical sampling aspects in the determination of the stopping power, and also to investigate empirical models that are customarily used to compute stopping power of compounds from that of the elementary constituents, e.g. the Bragg additivity rule.