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***Ab-initio* description of the electronic stopping power beyond the
Born-Oppenheimer approximation**

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Ever since the pioneering speculations in the 1960's about the multiple effects that a collision cascade produced by an energetic particle would induce in a solid target, there has been a huge interest in understanding the complexity of this highly non-equilibrium many-body electron-ion process in detail. In order to describe radiation damage in condensed matter, a tremendous amount of research effort – using both experimental techniques and computer simulations – has been fueled. Thereby, understanding the electronic stopping power, as the primary source of deposited energy, is of extreme significance for designing materials that withstand high levels of radiation damage caused by high-velocity ions (projectiles) produced by primary sources or by collision cascades.

However, the vast majority of computational research in material science, including the field of radiation damage, has been done within the adiabatic Born-Oppenheimer approximation. By assuming that the electrons adjust instantaneously to moving ions (e.g. by remaining in the ground state), this approximation amounts to that the quantum dynamics of the electronic system is completely ignored.

To overcome this drastic approximation, we present a newly-developed first-principles approach to address the electron dynamics. Our approach is based on the real-time propagation of the time-dependent Kohn-Sham equations and shows an excellent scalability. Thus, it is suitable for large-scale simulations involving several hundreds of electrons. After discussing our method in some detail, we show an important application by investigating the stopping of fast H atoms in bulk materials, such as Al and Cu.

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