

Electronic stopping power of molecular hydrogen in aluminum

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Synopsis Using time-dependent density functional theory and Ehrenfest dynamics to study the problem of electronic stopping of molecular hydrogen in aluminum. From this first principles non-linear dynamics approach we explore in details how velocity, orientation and geometry of the molecular hydrogen affects the electronic stopping power and how the dynamics of the interatomic distance affects the dissociation of the molecule.

When an object moves through a medium, it feels a *drag*, a force opposite to the movement direction. In some cases, a force perpendicular to the objects' velocity also appears. In the nanoscopic world, fast particles moving through a host material will feel a force due to interaction with host electrons. This is known as electronic stopping (S_e) [1]. These processes have received considerable attention in many applied fields of research, such as radiation therapies, accelerators, astrophysics and plasma physics [2].

In this work we focus on the simulation of electronic stopping of molecules. Since molecules are not spherically symmetric, new phenomena appear. In particular, the stopping force can be parallel to the velocity and additionally perpendicular to the velocity; the latter leading to electrodynamic lift. Additionally the orientation of the molecule with respect to its velocity can influence the stopping force.

The present calculations were done using Qball *ab-initio* code [3]. The initial system consist of the projectile (molecule) together with aluminum (108 atoms; with 3 valence electrons and the corresponding pseudopotentials associated with Al atom). The *xc* potential used in this study is due to Perdew-Burke-Ernzerhof (PBE) and periodic boundary conditions along with Eward summation were used in this study.

The projectile is initially placed in aluminum and a time-independent density functional theory (DFT) calculation was completed to obtain the converged ground state. We then performed time-dependent DFT (TDDFT) calculations on the electronic system with the moving projectile. The S_e is calculated from the average of the to-

tal force on the molecule as a function projectile distance [4, 5].

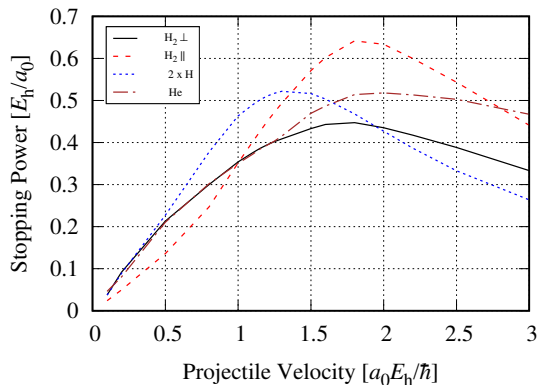


Figure 1. The S_e of projectiles (H, H_2 and He) in Al target as a function of projectile velocity. The solid (black) and dash (red) lines denotes the calculated S_e for H_2 projectile in \parallel and \perp directions respectively with $d = 2.0 a_0$. The dot (blue) and dash-dot (green) lines shows the results for H ($2 \times S_e^H$)

In summary, we have observed a new phenomena for the parallel and perpendicular orientation of the molecular hydrogen where there is a cross-over region at $v = 1.0$ a.u. with an interatomic distance of $2.0 a_0$. Also taking into account the dynamics of the interatomic distance yields good agreement with experimental data in terms of vicinage effect.

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