Eley–Rideal Recombination of Hydrogen on Tungsten (100) Surface: Isotope Effects and Energy Dissipation to the Surface.

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Adiabatic (BOSS) and nonadiabatic (LDFA-GLO) quasi-classical molecular dynamics simulations are performed to investigate the influence of isotopic substitutions and the energy exchange with the surface upon Eley–Rideal (ER) recombination of molecular hydrogen under normal incidence scattering of hydrogen isotopes on tungsten (100) surface.

Some of our results, like cross section and relative vibrational populations of the recombined molecules, are shown in these figures.

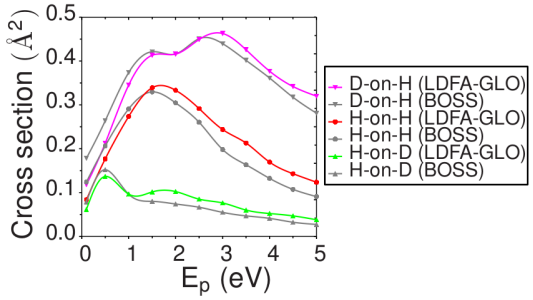

Figure 1: *ER recombination cross sections (in Å²) for some isotopic substitutions of hydrogen as a function of the initial energy of the projectile Ep (in eV), for BOSS and LDFA-GLO models.*

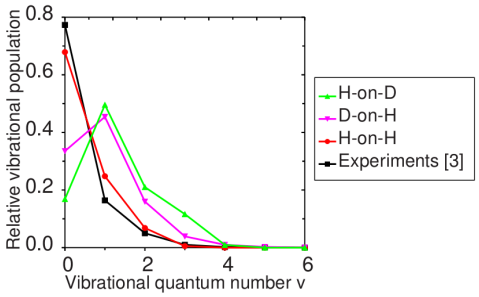

Figure 2: *Relative vibrational populations of the recombined molecules. Experimental results are in black square. Lines are drawn to guide the eye.*

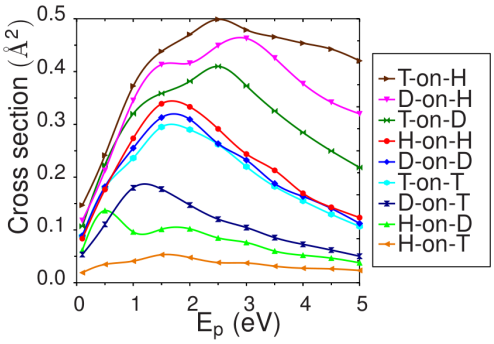

Figure 3: *ER recombination cross sections (in Å²) for all the isotopic substitutions of hydrogen as a function of the initial energy of the projectile, Ep (eV).*

The dynamics of this system depends on the mass ratio between projectile and target. The effect of including the energy exchange with the surface can be rationalized as a reduction of the effective collision energy. As a result, in the region where the ER cross sections increase (decrease) with energy, electronic excitations reduce (enhance) the recombination probability.

Index Terms: molecular dynamics, potential energy surface

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