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***Ab initio* molecular dynamics study of the dissosciation of H_2 on clean and hydrogen-covered Pd(100)** AXEL GROSS, Department of Theoretical Chemistry, University of Ulm, D-89069 Ulm, Germany — The adsorption of H_2 on the clean and hydrogen-covered Pd(100) surfaces has been studied by *ab initio* molecular dynamics simulations using density functional theory (DFT). In order to obtain statistically meaningful sticking probabilities as a function of the kinetic energy and the hydrogen coverage, about 150 trajectories of H_2 impinging on the surface have been computed per kinetic energy and hydrogen coverage. I have particularly focused on the role of the substrate atoms in the adsorption process. On the clean surface, the sticking probability is hardly influenced by the recoil of the metal substrate atoms because of the large mass mismatch. However, if the H_2 molecules impinge on a hydrogen-covered surface, the recoil of the preadsorbed hydrogen atom causes an significant enhancement of the sticking probability. This leads to a H_2 sticking probability which is much larger than what one would expect from a simple Langmuir kinetics picture.

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