NONREACTIVE SCATTERING OF N2 OFF W(100): RECONCILING EXPERIMENTS AND THEORY

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Résumé

The nonreactive scattering of N2 off W(100) is studied by means of quasi-classical trajectory simulations making use of a recently developed DFT-based potential energy surface (PES) relying on the vdW-DF2 functional. Dynamics are simulated within the Born-Oppenheimer Statistical Surface (BOSS) adiabatic approximation and the Generalized Langiven Oscillator (GLO) approach. The evolution of the widths of the in-plane scattering angle distributions, as a function of collision energy, shows a good agreement with experiments, in particular at low incidence energies. When allowing dissipation to surface motion within GLO, the scattering-angle-resolved final translational energies are also well reproduced. These results contrast with previous simulations using a PES based on the PW91 functional. The improvement is rationalized in terms of the topologies of both potential energy surfaces.

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