Supplementary Material (SM)

Modeling Surface Motion Effects in N$_2$ Dissociation on W(110): Ab Initio Molecular Dynamics Calculations and Generalized Langevin Oscillator Model

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These additional calculations presented as Supplementary Material are aimed to test the sensitivity of the results obtained with the generalized Langevin oscillator model (GLO) to the specific choice of parameters describing the surface and ghost oscillators, namely, the frequencies for parallel ($\omega_{x,y}$) and perpendicular motion (ω_z) and the friction coefficient associated to the ghost oscillator dynamics ($\gamma\, m_{\mathrm{W}}$, where m_{W} is the W atom mass). Taking $\omega_{x,y} = 19$ meV (7×10^{-4} a.u.), $\omega_z = 16$ meV (6×10^{-4} a.u.), and $\gamma = 6.6 \times 10^{-4}$ a.u. as the reference values, each test calculation is performed by varying one of the parameters while keeping the rest unchanged. For each parameter two test calculations are run that consist in either multiplying or dividing by a factor two its reference value in the case of the frequencies and by a factor 10 in the case of the γ. Figure S1 shows the results for the dissociation probability at normal incidence as a function of the collision energy. Similarly, the energy loss of the scattered N_2 as a function of the collision energy is shown in Fig. S2.
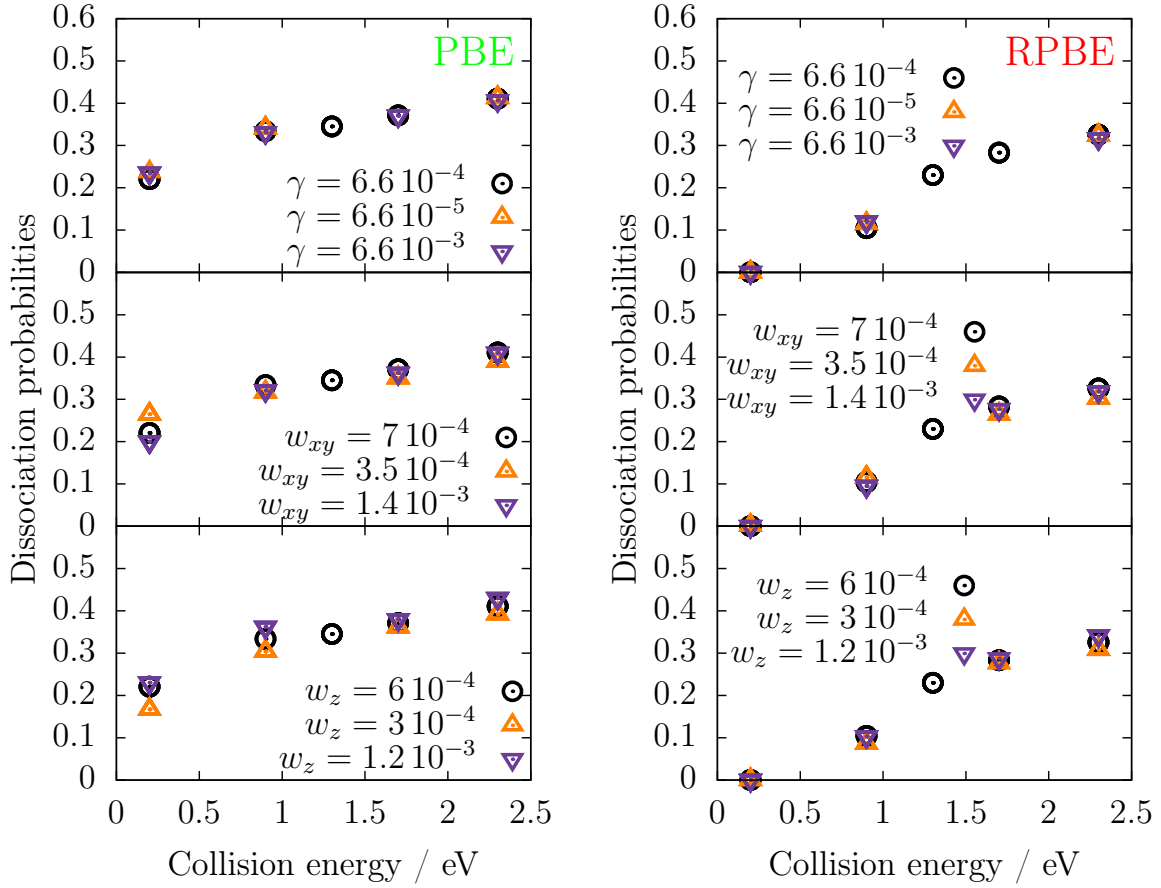
FIG. S1: Dissociation probabilities as a function of the collision energy obtained from quasi-classical GLO calculations using different values for the oscillator parameters. Left and right panels show the results obtained with the 6D PW91 and 6D RPBE PESs, respectively, when varying γ (top), $\omega_{x,y}$ (middle), and ω_z (bottom). In all cases, the results obtained with the reference values are plotted by the black-open circles. Calculations performed at normal incidence and for a surface temperature of 800 K.
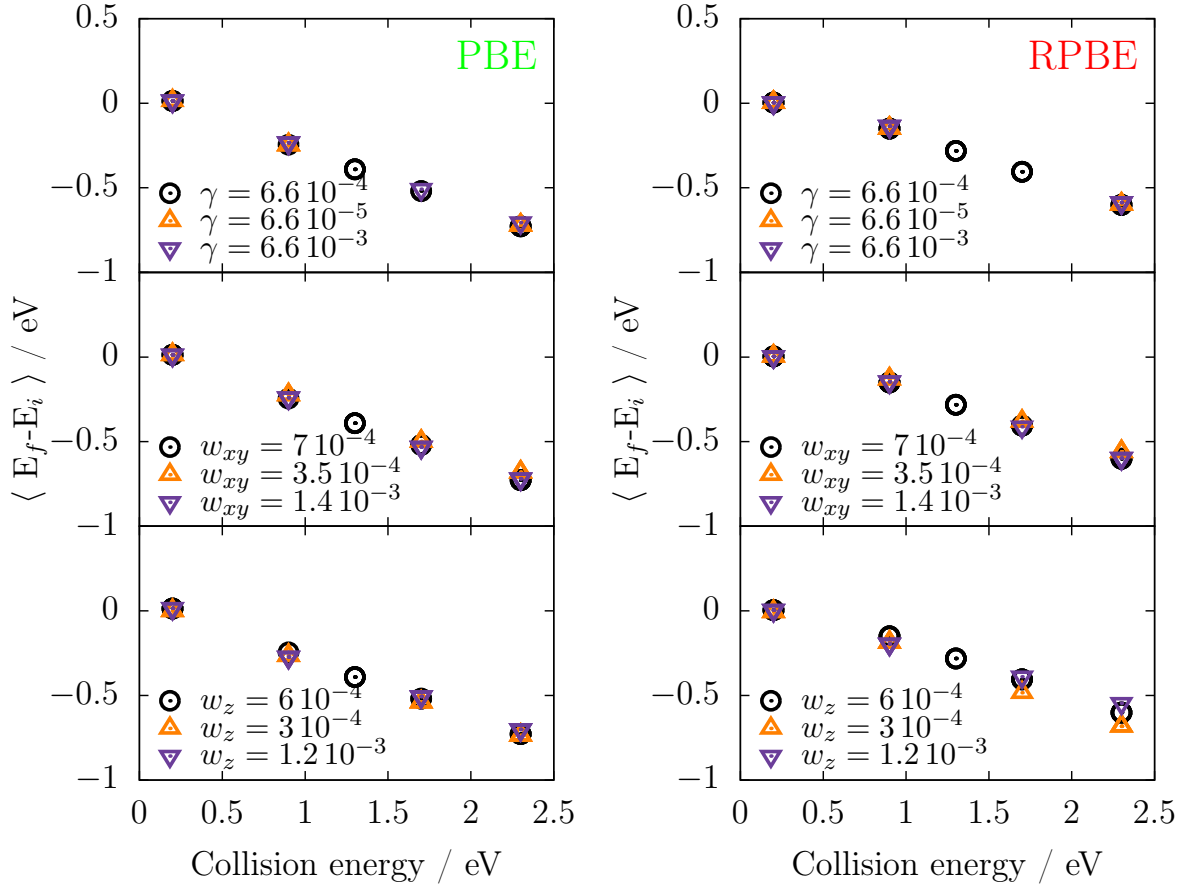
FIG. S2: Change in the total energy for the scattered N_2 molecules as a function of the collision energy. Results calculated with quasi-classical GLO calculations using different values for the oscillator parameters. Left and right panels show the results obtained with the 6D PW91 and 6D RPBE PESs, respectively, when varying γ (top), $\omega_{x,y}$ (middle), and ω_z (bottom). In all cases, the results obtained with the reference values are plotted by the black-open circles. Calculations performed at normal incidence and for a surface temperature of 800 K.