Analysis of reaction rates of single molecules on metal surfaces

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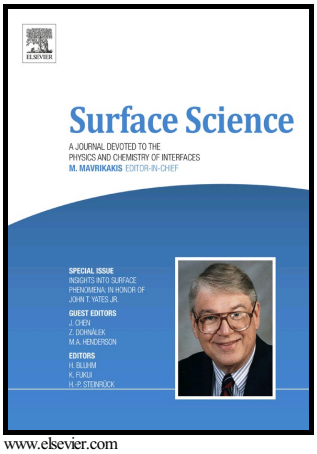

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Analysis of reaction rates of single molecules on metal surfaces

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Abstract

The experimental results of the action spectra *i.e.*,@reaction rate $R(V)$ as a function of a bias voltage V are analyzed for rotation of a single CCH (D) molecule on a Cu (100) surface [L. Lauhon and W. Ho, Surf. Sci. **451**, 291 (2000)] and hopping of a single $H(D)_2O$ molecule on Pd(111) surface [Fomin *et al*, Surf. Sci. **600**, 542 (2006)]. In the former system it is identified that rotation occurs if enough energy stored in the C-H (D) in-plane bending (IPB) mode excited by tunneling electron is transferred to the C-H (D) out of plane bending (OPB) mode (reaction coordinate mode) via the anharmonic mode coupling in a single electron process. The calculated $R(V)$ shows an excellent agreement with the experimental results except at the low bias voltages below $V \simeq 60$ mV where no experimental data is available for the nonlinear current I dependence of $R(I)$. A reproduction of the experimental $R(V)$ at the higher voltage region allows us to determine the vibrational density of states of the C-H IPB mode and its coupling rate to the C-H (D) OPB mode as well as the inelastic tunneling current to excite IPB mode. A change of a conductance upon excitation of the C-H IPB mode enables us to evaluate the electron-vibration coupling strength inducing the rotation motion of CCH molecule. In the latter system investigated at a high temperature of about 40 K, the constant $R(V)$ due to thermal hopping followed by the rapid increase is satisfactory explained by anharmonic inter-mode coupling between the scissor mode excited by tunneling electrons and the frustrated translation mode for $H(D)_2O$ molecule on Pd(111).