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Dynamics of STM-Induced Switching of Melamine/Cu(001) based on first-principles calculations TATSUHIKO OHTO, Department of Chemical System Engineering, The University of Tokyo, IVAN RUNGGER, School of Physics, Trinity College Dublin, KOICHI YAMASHITA, Department of Chemical System Engineering, The University of Tokyo, HISAO NAKAMURA, Nanosystem Research Institute (NRI), AIST, SANVITO STEFANO, School of Physics, Trinity College Dublin — The manipulation or stimulation of molecules using Scanning Tunneling Microscopy (STM) is a technique that recently has deserved deep attention for its potential applications in molecular electronics. The melamine/Cu(001) system was found to show switching behavior in very wide range of applied bias. Although its mechanism was analyzed by a statistic model, the relationship between the switching rate and bias is still far to be fully clarified. In this context, we performed a campaign of exhaustive first-principles calculations to obtain most of the parameters for resonance model; such model is able to predict the switching rate as functions of bias and current. The energy barrier was calculated using the nudged elastic band method, with the aid of recent implementation of current-induced forces into SMEAGOL code, which is based on the nonequilibrium Green's function method with Density Functional Theory. The electron-phonon coupling and then the Inelastic Tunneling Spectroscopy signal are calculated to validate the one-phonon approximation. The spatial distribution of molecular orbitals and their coupling with vibrational modes are very useful to understand the switching behavior.

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