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The dynamics of quantum tunneling: effects on the rate and transition path of OH on Cu(110) ERLEND DAVIDSON, University College London, ALI ALAVI, University of Cambridge, ANGELOS MICHAELIDES, University College London — The quantum tunneling of hydrogen is important to many scientific disciplines. Through well-defined experiments at surfaces with for example scanning-tunneling microscopy (STM) it is possible to understand the fundamental mechanisms involved at the atomic level. Recent STM experiments have identified OH on Cu(110) as an interesting model system in which the low temperature dynamics is entirely dominated by proton tunneling. Here we report the results from our analysis of the quantum nuclear tunneling dynamics of this system using density functional theory based techniques. We present computed classical, semiclassical and quantum mechanical transition rates for the flipping of OH between two degenerate energy minima. The classical transition rate is essentially zero at the temperatures used in experiment, and the tunneling rate along the minimum energy path is also much too low compared to experimental observations. However when tunneling is taken into account along a direct path connecting the initial and final states with only a small amount of the oxygen movement the transition rate obtained is in much better agreement with experiment, suggesting quantum tunneling effects cause a deviation of the reaction coordinate from the classical transition path.

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