

# DIRECTIONAL PREFERENCE ON CU(110)

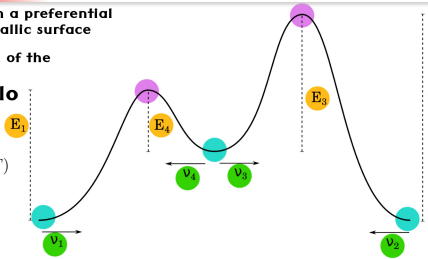
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\* Looking for molecules with a preferential diffusion direction on a metallic surface

\* Simulation of the diffusion of the molecules on Cu(110) via

**kinetic Monte Carlo**

$$k = \frac{\prod_i^{3N} \nu_i^{min}}{\prod_i^{3N-1} \nu_i^{sad}} \exp(-E_s/k_B T)$$



**Geometry Optimization**

Minima

Transition states

Nudged Elastic Band

Dimer Method

Frequency calculations

