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Diffusion of Small 2D-Cu Clusters on Cu (111)[1] ALTAF KARIM, AHLAM N. AL-RAWI, ABDELKADER KARA, TALAT S. RAHMAN, Department of Physics, Kansas State University — Diffusion of small Cu clusters containing 2 to 10 atoms on Cu (111) has been studied in detail using Kinetic Monte Carlo (KMC) and molecular dynamics simulations (MD). Our KMC simulations are based on a comprehensive database including more than 500 mechanisms for cluster diffusion and their related energetics calculated using embedded atom potential method. The MD simulations, at 500K and 700K, have been instrumental in revealing several mechanisms for cluster diffusion especially those involving concerted motion of several atoms. From the calculated diffusion coefficients at 300K, 500K, and 700K, we find that the effective diffusion barriers increase almost monotonically with increasing cluster size. The inclusion of the newly revealed mechanisms from MD in our KMC simulations thus negates an earlier finding of magic cluster sizes. Contrary to the case of larger clusters (20 to 1000 atoms), we do not find a simple scaling of the diffusion coefficient with cluster size.

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