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Diffusion Prefactors and Vibrational Entropic Contributions for small Cu and Ag clusters on Cu(111) and Ag(111)[1] HANDAN YILDIRIM, ABDELKADER KARA, TALAT S. RAHMAN, Department of Physics, University of Central Florida — In examination of the diffusion energetics and dynamics of small 2D Ag and Cu clusters on Ag(111) and Cu(111) we found the results for the 7-atom cluster to be particularly interesting. In particular the diffusion pre-exponential factor for the Cu clusters on Ag(111) is found to be one order of magnitude larger than that for the homo-systems; Cu cluster on Cu(111) and Ag cluster on Ag(111). Analysis of the vibrational entropic contributions to the system free energy points to the subtle differences in the three cases and the significant contribution of the substrate atoms that lie in the vicinity of the diffusing islands. We trace the differences in the results for the 7-atom cluster from those for smaller sized ones to the nature of the cluster-substrate interactions. The vibrational dynamics and energetics of the systems are obtained using ab initio electronic structure calculations (density functional theory) and compared to those obtained using many body interaction potentials.

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