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Enhancement of Ag Cluster Mobility on Ag(111) Surface by clustering with Chlorine[1] YU-NING WU, HAI-PING CHENG, Department of Physics and Quantum Theory Project, University of Florida, USA, NOUARI KEBAÏLI, ALBERT MASSON, CATHERINE BRÉCHIGNAC, Laboratoire Aimé Cotton, CNRS-Université Paris Sud 11, France — Chlorine is observed to accelerate the fragmentation of Ag nanostructures deposited on graphite. To understand the role of chlorine in the stability of Ag nanostructures, we have studied the formation and diffusion of Ag_n and Ag_nCl_m (n= 1 to 4) clusters on Ag(111) surface, using density functional theory (DFT) with generalized gradient approximations (GGA) and the projector-augmented wave method. Our calculation shows that the formation energies and diffusion barriers of Ag_n clusters are both lowered by clustering with chlorine when n=1, 3 and 4, indicating the enhancement of mass transport on Ag(111) surface. $(AgCl)_n$ clusters (n=1, 3 and 4) are good candidates for surface mass transport units. We have also studied a chloridized Ag_{55} cluster and an Ag_{55}-Ag_{55} neck structure. Chlorine is found to loosen the Ag_{55} structure and weaken the binding between the Ag_{55} bulbs in the neck structure.

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