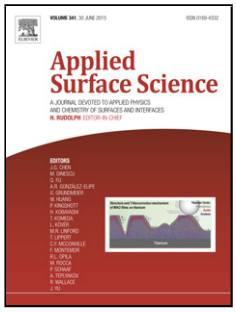

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Structures and stabilities of small Co clusters on a Cu(111) surface: a theoretical study

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Abstract: Structures and relative stabilities of small Co_n clusters (n=1~12) on a Cu(111) surface are studied using molecular dynamics simulations. It is shown that the supported clusters are all in two-dimensional island structures of the edges forming square microfacets (A step) and/or triangular microfacets (B step) with the substrate. For non-magic-number clusters, the lowest energy structures are the ones of the edges with more A steps and the most unstable structures are the ones of the edges with only A steps or B steps due to the lattice mismatch of the Co_n/Cu(111) system. Magic number clusters are truncated triangular or elongated shapes with a closed atomic shell and maximum nearest-neighbor bonds. In addition, the anomalous mobility is found for Co_3 and Co_6 clusters in the diffusion processes of these clusters. The concerted translation and rotation movements are responsible for their special diffusion behaviors.

Keywords: Metal surface; Molecular dynamics; Cluster structure; Cluster diffusion.

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