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Magic planar Ag clusters Y.P. CHIU, C.M. WEI, C.S. CHANG, TIEN. T. TSONG, DEPARTMENT OF PHYSICS, NATIONAL SUN YAT-SEN UNIVERSITY, KAOHSIUNG, TAIWAN, ROC COLLABORATION, INSTITUTE OF PHYSICS, ACADEMIA SINICA, TAIPEI, TAIWAN, ROC COLLABORATION, INSTITUTE OF ATOMIC AND MOLECULAR SCIENCES, ACADEMIA SINICA, TAIPEI, TAIWAN, ROC COLLABORATION — The spontaneous assembly of atoms and molecules in a system has attracted many research interests and created numerous potential applications. Utilizing the periodic pattern found on the Pb quantum islands, which are grown on the Si(111) surface, we have recently discovered that self-organized Ag planar clusters formed on these templates exhibit enhanced stability at some particular sizes. Detailed calculations based on ab initio density functional theory have also been performed. The use of a density-functional optimization in geometrical structures and the corresponding binding energy support an examination of the genesis of these magic Ag nanoclusters and their relative stability. When the Ag nanopuck grows to a certain size, the geometrical effect takes hold from the electronic effect as the major attribute, which drive the Ag nanopucks towards well defined hexagonal crystalline structures. The theoretically related electronic and geometrical structures are also correlated with the experimentally energetically favorable structures of these magic clusters.

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