

Abstract Submitted
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Selective self-assembly of molecular clusters with designed sizes on metal surfaces¹ JUN WANG, QING LI, MIGUEL FUENTES-CABRERA, BOBBY G. SUMPTER, ARTHUR P. BADDORF, MINGHU PAN, Oak Ridge National Laboratory — The self-assembly of “magic” molecular clusters on various substrates provides a new arena for studies of surface nanocatalysis and molecular electronics. Here we present the self-assembly of phenylacetylene molecules on Cu(100) by a combined low-temperature STM and in-depth density functional theory investigation. We observe the molecules form distinct tetramer clusters on Cu(100) at 40 K. Each cluster has a four-fold symmetry and consists of four molecules. A delicate balance of intramolecular and dipole-dipole interactions between clusters maintains this magic tetramer configuration on Cu(100). The strong interaction between the molecules and the copper surface creates an anchor at each adsorption site. Through comparison with our previous observed hexamer (six-molecule) clusters on Au(111), we conclude that the epitaxial relationship between the molecules and metal surfaces is crucial in defining magic numbers of surface-supported molecular clusters under weak intermolecular interaction.

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