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First-Principles Study of One-Dimensional Metal-Molecule Hybrid Chains Self-Assembled on Ag Substrate BON-GIL KOO, YOUNG-KYUN KWON, Department of Physics and Research Institute for Basic Sciences, Kyung Hee University — We explore the formation mechanism and the structural and electronic properties of one-dimensional metal-molecule hybrid chain self-assembled on Ag(111) substrate using *ab initio* density functional theory. It is observed that such a hybrid chain is formed by spontaneous transformation from 4,4"-dibromo-*p*-terphenyl (DBTP) molecules when deposited on Ag(111) substrate at room temperature. We find that the chain is composed of *p*-terphenyl (TP) connected through an Ag atom to form $(\text{TP-Ag})_n$. Our study shows that Ag(111) surface plays a catalytic role removing two Br atoms (DB) from DBTP and connecting the remaining TP through an Ag atom, which is a similar phenomenon as the Ullmann cross coupling reaction occurred on Cu surface. We find that those Br atoms detached from DBTP play important roles for spontaneous formation of well-aligned pattern. Our calculated electronic structures and simulated scanning tunneling microscopy (STM) images of $(\text{TP-Ag})_n$ hybrid chain exhibit remarkably different charge distributions depending on the energy values, which are related to the tip voltage in STM experiments. We also investigate the end state of the hybrid chain, which can be spatially resolved.

Young-Kyun Kwon
Department of Physics, Kyung Hee University

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