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The formation of conductive polymer chains from Biphenyl-4,4'-dithiol (BPDT) molecules on rough Ag surfaces[1] RUQIAN WU, V. ARA APKARIAN, University of California, Irvine, YANNING ZHANG, Chengdu Green Energy and Green Manufacturing Technology Research and Development Center — Single-molecular electronics, which exploits novel physical and chemical properties of organic molecules, has attracted much attention in the last decade. Many experimental and theoretical efforts have been made in manipulating high-quality organic polymers, understanding electron transport properties and developing electronic devices. Our experiments show that self-assembled monolayer (SAM) of Biphenyl-4,4'-dithiol (BPDT) can readily form on roughened surfaces of elemental silver, instead of a flat surface. To understand "why so," we performed systematic density functional studies on the structural, energetic and electronic characteristics of both isolated BPDT molecules and BPDT on Ag(111) surfaces, with the inclusion of van der Waals correction in DFT. The formation of S-Ag-S linkage makes the molecule chain metallic, different from the insulating feature of S-S linkage. The adsorption of BDPT on roughened Ag surface is energetically preferred compared to that on flat surface. Moreover, the Ag adatom makes BPDT molecules attractive to each other on Ag(111) surface, crucial for the formation of polymer chains. Our joint theoretical and experimental results indicate the feasibility of fabricating conductive organo-silver polymer sheets.

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