

Abstract Submitted
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Tailoring

thermopower of single-molecular junctions by temperature-induced surface reconstruction¹ CHIUNG-YUAN LIN, Department of Electronics Engineering, National Chiao Tung University, BAILEY HSU, Department of Electrophysics, National Chiao Tung University, YAU-SHIAN HSIEH, Department of Electronics Engineering, National Chiao Tung University, YU-CHANG CHEN, Department of Electrophysics, National Chiao Tung University — Recent experiments revealed that surface reconstruction occurs at around 300-400K in the interface of C₆₀ adsorbed on Cu(111) substrate by scanning tunneling microscope techniques. To understand effects of such reconstruction on thermopower, we investigate the Seebeck coefficients of C₆₀ single-molecular junctions without and with surface reconstruction as a function of temperature at different tip-to-molecule heights from first-principles. Our calculations show that surface reconstruction can enhance or suppress Seebeck coefficients according to junctions at different tip heights. We further observe that the Seebeck coefficient of the junction at $d = 3.4\text{\AA}$ may change from p- to n-type under surface reconstruction.

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