

论文

电极距离和外部电压对“金 / 有机分子 / 金”三明治型隧道结的电子传输特性影响

轩书科

山东工艺美术学院公共课教学部, 山东 济南 250300

摘要:

以“金 / 1,4-二氰基甲苯分子(C₆H₄(CN)₂) / 金”隧道结为研究对象,从第一性原理出发,计算了电极距离和外部电压2个因素对隧道结电子隧穿特性的影响。隧道结的开启电压随电极距离的变化不是单调的,从1.278nm到1.298nm,开启电压减小;从1.298nm到1.398nm,开启电压增大。外部电压导致界面处的电荷积累会阻碍电子的隧穿。理论计算的电流、电导曲线和实验曲线符合较好。

关键词: 电子传输 隧穿结 电极距离

The effects of bias voltage and the distance between two electrodes on the transport properties of the Au / molecule / Au junctions

XUAN Shu-ke

Common Course Teaching Department, Shandong University of Art & Design, Jinan 250300, Shandong, China

Abstract:

Based on the first principle calculation method, the effects of bias voltage and the distance between two electrodes on the transport properties of the Au / molecule / Au junctions was investigated. The bias voltage corresponding to the first onset of the conductance decreases with the electrode distance from 1.278nm to 1.298nm, and increases with the electrode distance from 1.298nm to 1.398nm. The electron accumulation at the interface between molecule and electrode resulting from the bias can hamper electron tunneling. Good agreement between calculation results and experimental results in conductive features was achieved.

Keywords: electron transport tunnelling junction the distance between electrodes

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作者简介:

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