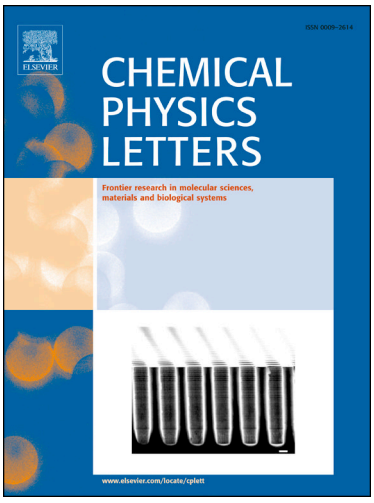

Research paper

Pyridine "alligator-clip" as molecular negative differential resistor predicted by first-principles study

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Pyridine "alligator-clip" as molecular negative differential resistor predicted by first-principles study

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Abstract

Based on non-equilibrium Green's function and density functional theory, a first-principles study of the transport properties of two benzene-pyridines sandwiching the σ barrier of ethyl is performed. Using symmetric leads, strong negative differential resistance (NDR) effects with high peak-to-valley ratios (PVRs) are present under low bias. When using asymmetric leads, the PVR can be modulated to higher value with the unchanging of voltage (V_{peak}) corresponding current peak (I_{peak}). Our investigations indicate that pyridine "alligator-clip" can be used as very good low bias molecular NDR devices.

Keywords: Molecular electronics; Negative differential resistance; First-principles; Non-equilibrium Green's function; Density functional theory

1. Introduction

NDR effect is that the current decreases as bias increases in a certain bias region. The traditional electronic device with NDR effect is Esaki or resonant tunneling diode (RTD) [1] and has many applications such as analog-digital converters, high-frequency oscillators, and logic circuits.[2-4] The standby power of Dynamic Random Access Memory (DRAM) can be reduced significantly if the RTDs are used. Molecular NDR devices are very valuable because they are considered as potential substitute of compound (III-V) semiconductor [5] for realizing memory cells with extremely low static power dissipation and very high density. Recently, as other molecular devices, molecular NDR devices [6-36] have attracted many investigational interests. Among these researches, most molecular NDR effect presents in high bias region. A few molecular NDR effect presents in low bias region but the PVR (the ratio between current peak and current valley) is not large enough. There has been investigations [37] pointed out that if the molecular NDR devices were used for local refresh of DRAM memory cells, they should present the NDR effect under low bias and have large PVR value. In a word, low bias molecular NDR devices with large PVR are valuable in the future. Here, a first-principles study of the transport properties of the σ barrier separating two benzene-pyridine molecules sandwiched between Au or Ag leads are performed. The