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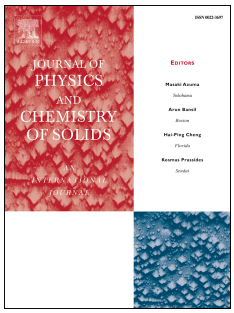

Low bias negative differential resistance in tour wires predicted by first-principles study

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Low bias negative differential resistance in Tour wires predicted by first-principles study

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Abstract

Tour wires are considered as potential block materials for molecular electronics in the future. This work provides a first-principles study of the transport properties of three Tour wires sandwiched between two Al leads by pyridine "alligator clip" connecting apex Al atom. We obtained strong negative differential resistance (NDR) effect under very low bias and such NDR effect can be modulated by the length of the Tour wire, which promise the potential applications in molecular devices in the future.

Keywords: First-principles; Molecular electronics; Tour wire; Negative differential resistance

Introduction

For trying to replace the traditional semiconductor-based devices with molecular-based counterparts, molecular electronics (ME) recently attract much investigational interesting. From the aspect of fundamental research, the ME can help one to understand how the charge transport along molecules below nano-scale [1, 2]. From the aspect of applications, the ME can potentially realize the ultimate miniaturization of electronic devices [3]. Seeking excellent molecules for the ME is one of important missions for investigators. Tour wires [4] are a kind of molecular wires which consist of tripled bonded carbon atoms separating phenyl rings and form long rigid molecules with π-conjugated delocalized frontier orbitals. Such molecular wires can be synthesized as long oligomers and have become outstanding building blocks for molecular devices. Several research works [5-11] found the negative differential resistance (NDR, a nonlinear electrical phenomenon that the current decreases as bias increases in a certain bias region and has important applications in logic, analog-to-digital converters and oscillators [12-14]) in the molecular devices based Tour wires. Among these researches, the peak-to-valley ratio (PVR, the ratio between current peak and current valley) of some NDR effects is not large enough. Even if some NDR effects have very large PVR, the bias region where the NDR effects locate is very high. There is a study work [15] has indicated that the molecular NDR effect should has potentially application value only if it is under low bias region. In addition, low bias NDR effect means low power dissipation. For these reasons, low bias molecular NDR devices are significant. In present work, we perform a first-principles study of the transport