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**Negative differential resistance (NDR)  
of ferrocenyl-alkanethiolate on the Au (111) surface** SHUCHUN WANG,  
NC State U., WENCHANG LU, QINGZHONG ZHAO, JERRY BERNHOLC —

With the rapidly growing interest in the development of molecular electronics, the resonant tunneling diode (RTD) becomes an attractive molecular device goal due to its utility in switching logic and simplicity in integration. Molecular systems displaying Negative Differential Resistance (NDR) and resonant tunneling show great potential as RTDs. In a recent experiment, self-assembled monolayers (SAMs) of ferrocenyl-alkanethiolate on gold show clear molecular NDR, but its mechanism has not been identified. We report first-principles studies of electronic transport in such SAMs by the non-equilibrium Green functions method. The calculated I-V characteristics show strong NDR at both positive and negative biases, which are in good agreement with the experimental results. We find that the ferrocene group acts like a quantum dot and that the resonant coupling between its HOMO and the gold leads is responsible for the NDR features. Such molecules could lead to novel RTDs in nanoscale molecular devices.

Shuchun Wang

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