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TÉMA

Single-Molecule Charge Transport Studies on Nanocarbon Materials

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Understanding charge transport through nanocarbon materials across the metal–molecule interface is a fundamental issue in organic devices. In recent years, single-molecule scale studies on charge transport through the metal–molecule interface have been made possible by break junction techniques. Here, we present our recent single-molecule transport studies on nanocarbon materials using scanning tunneling microcopy (STM) and break junction techniques in combination with current-voltage measurements and fist principle simulations [1-4].

Bowl-shaped π-conjugated nanocarbons, or buckybowls, are a novel class of sp2-hybridized nanocarbon materials. In contrast to tubular carbon nanotubes and ball-shaped fullerenes, the buckybowls feature structural flexibility. Bowl-to-bowl structural inversion is one of the unique properties of the buckybowls in solutions. Bowl inversion on a surface modifies the metal–molecule interactions through bistable switching between bowl-up and bowl-down states on the electrode surface, which makes surface-adsorbed buckybowls a relevant model system for elucidation of the mechano-electronic properties of nanocarbon materials. We demonstrate that the bowl inversion can be induced by approaching the STM tip toward the molecule. By tuning the local metal–molecule interaction using the STM tip, the sumanene buckybowl exhibits structural bistability with a switching rate that is two orders of magnitude faster than that of the stochastic inversion process.

Aromaticity of nanocarbons is a fundamental concept in chemistry. Antiaromatic nanocarbons are predicted to exhibit remarkable transport properties and high redox activities. However, it has only been possible to measure compounds with reduced aromaticity but not antiaromatic nanocarbons due to their energetic instability. We addressed these issues by investigating the single-molecule charge transport properties of a genuinely antiaromatic nanocarbon, showing that antiaromaticity results in an order of magnitude increase in conductance compared with the aromatic counterpart. Single-molecule I-V measurements and first principle transport calculations reveal that this results from a reduced energy gap and a frontier molecular resonance closer to the electrode potential in the antiaromatic species. The conductance of the antiaromatic complex is further modulated electrochemically, demonstrating its potential as a high-conductance transistor.

References

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