ELASTIC QUANTUM TRANSPORT FOR MOLECULAR NANOSWITCHES USING PLANE WAVES

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Molecular electronics represents an interdisciplinary area that spans physics, chemistry and material science, and is based on the use of molecular building blocks for the fabrication of electronic components. In recent years, new advances have made possible a real technology based on molecular electronic devices, such as rectifiers, resonant tunnel junctions and molecular switches. The later refer to electronic switching devices that use molecules as active components, and have been extensively studied these years. Switching behaviour has been observed in different species and various schemes have been suggested to describe the physical origin of the molecular switching processes.

In this work, the switching behaviour of phenyl-based molecules attached to copper electrodes through thiol end groups is investigated, where the switching is driven by conformational changes involving the rotation of one of the phenyl groups. The elastic quantum transport of such nanodevices is calculated using a recently developed numerical method.[1,2] This method is based on a solution of scattering states using plane waves and auxiliary periodic boundary conditions, includes evanescent states exactly, and its computational time is close to that of a ground-state DFT calculation. To test the accuracy of this approach, a benching mark problem is first considered, which consists of a di-thiol benzene (DBT) molecule connected by two Cu wires.

Subsequently, di-thiol biphenyl and di-thiol biphenyl-acetylene molecular devices have been studied. For each molecular nanosystem two different configurations are considered, with phenyl rings either lying on the same plane or rotated 90 degrees with respect to each other. Compared to the result for the DBT molecule, the zero-bias conductance is not significantly affected by the inclusion of a second coplanar phenyl ring (ON state), whereas rotating one phenyl ring drops the conductance greatly (OFF state). As a result, large ON-OFF ratios are found by simple rotation of one of the benzene molecules.

The approach presented here provides a computationally inexpensive and accurate way to methodically describe switching behaviour of molecular nanodevices, and work is in progress for its implementation to non-zero applied bias voltages, which require a non-self consistent treatment of the out-of-equilibrium situation.

References

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