Small carbon clusters as molecular switches: modeling and working principles

D.A. Luzhbin

Institute for Metal Physics, National Academy of Sciences of Ukraine, Kyiv, Ukraine

Recent molecular dynamics simulations[1] have predicted existence of the smallest carbon fullerene C8, which has an extremely long lifetime at low temperatures. An example of a molecular current switch built of a single C8 molecule attached to gold electrodes is considered and its zero-temperature electronic and transport properties are calculated from the first principles. It is shown that zero-bias conductance of the switch depends nonlinearly on the length of the junction and develops a sharp drop of an order of magnitude for some particular length.[2] Current-voltage characteristics of the switch can show either metallic or semiconducting behavior depending on the length of the molecular junction. By tuning the value of interelectrode separation one can change the properties of the junction in a quite wide range from a highly conducting metallic state to a super insulating state, where in a wide range of applied bias voltages the ratio of the currents in these two states exceeds 30. These particular properties can be used for constructing temperature switches whose sensitivity to the temperature changes reaches down to millikelvins. The specific details of the electronic spectrum of the junction, which are important for constructing C8 based molecular switches, are also discussed.

[1]L.A. Openov and V.F. Elesin, JETP Lett. **68**, 726 (1998).
[2]D.A. Luzhbin, Proc. 2nd Int. Sci. Conf.: Nanostructured Materials-2010 (NANO-2010), Oct. 19-22, 2010, Kyiv, Ukraine.