A lattice-induced attraction between lithium ions

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Normally ions with the same charge repel each other, but in very rare cases an intervening medium can produce an apparent attraction. By means of periodic DFT (density functional theory) calculations, we have found an apparent attraction between two lithium ions through a semiconducting CNT (carbon nanotube). Our results are in agreement with previous publications showing evidence that a lattice of carbon atoms can induce an apparent attraction between Li ions [1,2].

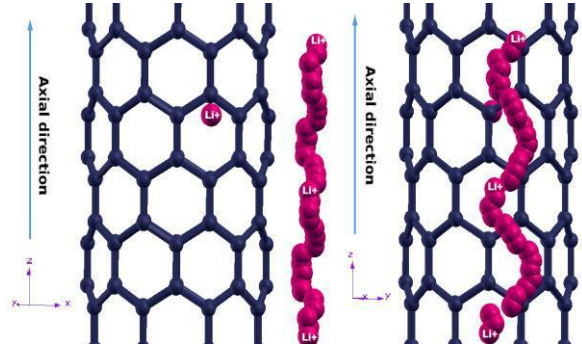

Fig. 1. Lateral and front view of (8,0) CNT with 2 lithium ions, one inside and one outside, showing the optimal path that the ion outside fallows in its z-coordinate.

In this work the interaction between 2 lithium ions (one inside another outside) and the CNTs has been modeled using plane waves. To address different electronic properties we have studied: (8,0) semiconducting, and (5,5) conducting nanotubes.

When the lithium ions adsorbs on the CNTs there is no chemical bond between them. Both Li atoms pass one electron each to the tube, creating an image or polarization charge. This effect produces a shift in the Fermi level in the vicinity of the lithium ion, and in the case of the semiconducting tube, it becomes conducting. When the second lithium is placed outside, the energy required to accept the second electron and to form the image charge is less, since there already is a substantial density of electrons at the Fermi level.

To observe this apparent attraction between the cations is important to use a material that suffers a major change in the occupation of its conduction band. This condition rules out metal or conducting tubes or layers, because their density of states at the Fermi level is too high.

1. Martin Z. Bazant, Brian D. Storey, and Alexei A. Kornyshev, Phys. Rev. Lett, **2011**, 106, 046102-2-046102-4
2. E.P.M. Leiva, E. Perassi, D. Barraco, Electrochemistry Comm, **2016**, 65, 48-52