Layered Ferroelectricity: from Geometric Measures to First-Principles Calculations

Oded Hod

School of Chemistry and The Sackler Center for Computational Molecular and Materials Science, Tel Aviv University, Tel Aviv 6997801, Israel.

Email address of corresponding author: odedhod@tauex.tau.ac.il

The ability to locally switch confined electric polarization is vital in modern technologies, aiming to complement or replace traditional magnetic components toward storing, retrieving, and processing large volumes of information. Non-centrosymmetrically stacked layered materials have recently emerged as promising candidates for vertical polarization switching via lateral interlayer shifts – a mechanism known as slidetronics.[1-5] In this presentation, I will elucidate the microscopic origins of polarization in layered materials; demonstrate that it is dictated by interlayer registry; explain its cumulative nature and its saturation behavior; show that it can emerge also in intrinsically non-polar systems, such as graphitic interfaces; and extend the notion of slidetronics to the quasi-one-dimensional case of facetted nanotubes (see Fig. 1).

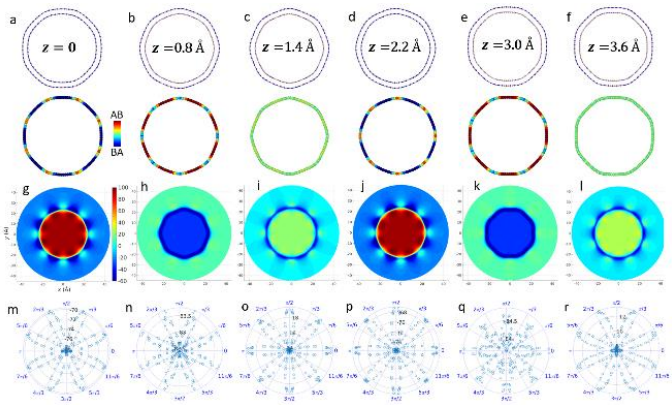

Fig. 1. Axial interwall shift induced superstructure and radial polarization variations calculated for a zigzag (55,0)@(63,0) double walled boron nitride nanotube (DWBNNT) of preoptimized inner and outer wall diameters of 43.8 Å and 50.2 Å, respectively. (a)-(f) Cross-sectional views of the relaxed DWBNNT for several coaxial shifts, z=0, 0.8, 1.4, 2.2, 3.0, and 3.6 Å. In each panel, the upper illustration represents the atomic structure and the lower illustration superimposes the corresponding local polarization registry index map on the outer wall atomic positions (see color bar in panel a). (g)-(l) Density functional theory calculated electrostatic potential difference maps (with respect to the same individual walls) plotted along the (001) face of the DWBNNTs presented in panels a-f, respectively. The color bar appearing in panel g is common to panels h-l. (m)-(r) Polar diagrams presenting the difference in electrostatic potential (in meV) calculated outside the tube at a radius of r=35 Å and inside the tube at a radius of r=5 Å. These values are obtained for each angle by radially averaging over a range of 0.02 Å and axially averaging over the length of the unit cell.

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