Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Reversible Actuation of a-Borophene Nanoscrolls

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SUPPLEMENTARY INFORMATION

1. Molecular Dynamics Simulation Videos File

There are four video files:

1- zz-heat-charge-cool.mp4
2- ac-heat_charge_cool.mp4
3- zz_molecular.mp4
4- ac_molecular.mp4

All files contain simulations carried considering the DFTB approximation as implemented in DFTB+ software. For the description of boron atoms and their interatomic interaction, we adopted the Borg parametrization, as explained in the article. The aim of these simulations is to to exemplify the unrolling process triggered by charge injection on these materials, as explained throughout the text. ac-heat-charge-cool.mp4 file contains the visualization of the trajectory obtained during the simulation of a boron nanoscroll unitary cell rolled up along the “Armchair” direction, while zz-heat-charge-cool.mp4 refers to a similar simulation carried for a “Zigzag” boron nanoscroll unit cell. Files zz_molecular.mp4 and ac_molecular.mp4 show similar simulations considering non-periodic nanoscrolls, with charge injection/atom similar to that used in the periodic cases. In both cases the same simulation protocol was applied as follows:

1- Linear heating from 10K up to 600K;
2- Approximately 0.03 electrons/atom injection into the system at 600K, triggering the unrolling process;
3- Extraction of charges followed by a linear cooling down to 300K.

It is interesting to note that the periodic “zigzag” nanoscroll re-rolls completely at the end of the process, while the “armchair” nanoscroll doesn’t, revealing an important effect of the rolling up axis direction on electro-actuation effects.

In the case of molecular simulations we have also shown that, after charge injection, the nanoscroll unrolls and, after charge removal it starts to re-roll in both cases.

2. **DFTB Keywords and Considerations for the Simulation**

   a. **Optimization**
   Optimizer - Rational
   LatticeOpt - Yes
   Convergence - GradElem = 1.0E-05 Hartree/Bohr

   b. **Hamiltonian and SCC calculations**
   SCC - Yes
   SCCTolerance = 1.0E-7
   MaxAngularMomentum - B = “p”
   Filling - Fermi - Temperature[Kelvin] = 300
   Dispersion - LennardJones - UFFParameters
   SlaterKoasterFiles - borg-0-1
   KPointsAndWeights - SupercellFolding - 1 (0.0) x 8 (0.5) x 1 (0.0)
   Charge[e] = 0 to +15

   c. **Thermostat(for MD simulations)**
   Thermostat: Nose-Hoover
   Coupling Strength = 3000

3. **Distance Definition of distance between nanoscroll tips:**

   As explained in the main text, distances between tips were calculated considering the mean (y,z) position of those tips for zigzag and the mean (x,z) position of the armchair nanoscroll tips. Using the definition above we have a well defined distance between the line of atoms in one tip to the equivalent line on the other tip. In our calculations, the relative variation of (x,z) and (y,z) positions were considerably small, being typically under 1.0%.

4. **Information about the python codes**

   There are two python code files:

   1- gen-scrolls-quasi-2d-graphical.py
   2- gen-scrolls-quasi-2d-text.py

Both are constructed to perform the rolling up of a sheet placed at xy, xz or yz plane. The rolling is made around the x, y or z axis following an archimedean spiral with interlayer distances defined by the user.

The difference between these two codes is only cosmetical, namely the first one (gen-scrolls-quasi-2d-graphical.py) comprises a simplified graphical interface, while the second (gen-scrolls-quasi-2d-text.py) has only a simple text interface.

PS: Initial configuration files with the explicitly “xyz” coordinates for both systems are available upon request.