Electrostatics and/or elastic optimal arrangement of triangular lattices confined to cylindrical fibers

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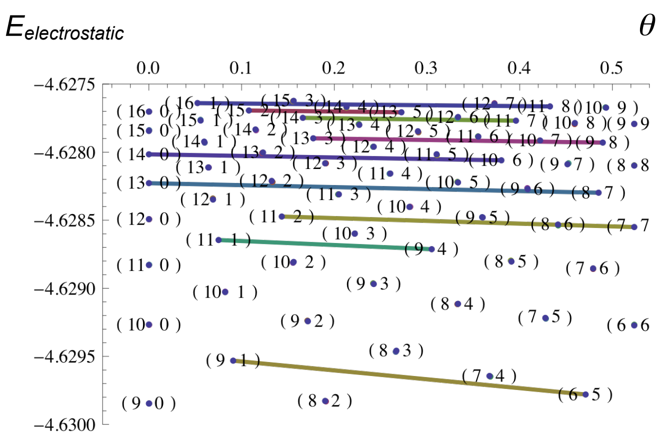
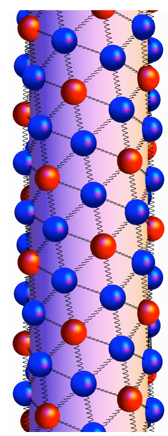
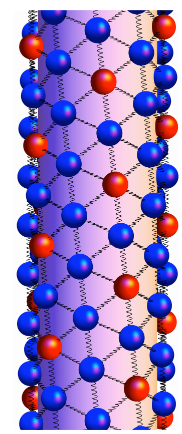
The optimal arrangement of triangular lattices wrapped around the surface of a nanofiber is computed to determine the effects of surface curvature on the orientation of the lattice. The authors find electrostatic interactions favor *chiral* arrangements only for special families of lattices dependent on the fiber diameter. However, certain families of lattices promote energetically favorable zig-zag *achiral* configurations. They further consider the behavior of short-range elastic forces, represented by interconnected springs between neighboring sites. For this case, as well as other short-range interactions, including van de Waals, the *achiral* armchair lattice family is always preferred. Such a scenario appears to be stable for highly curved nanotubes, and it is not modified significantly by varying the stoichiometric composition of charges or by the inclusion of higher-order curvature effects.

Zig-zag lattices

- Fibers of charge ratios tiled with *2:1 ionic lattices* prefer zig-zag (*p, p*) conformations (left plot)
- Chiral (p_1, p_2) configurations are preferred only in special cases of fiber diameters

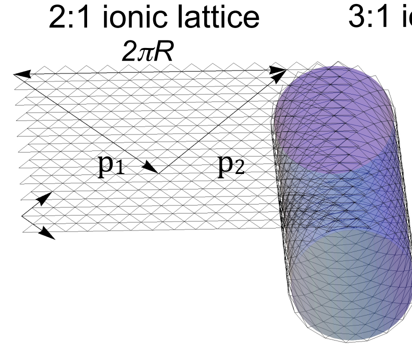


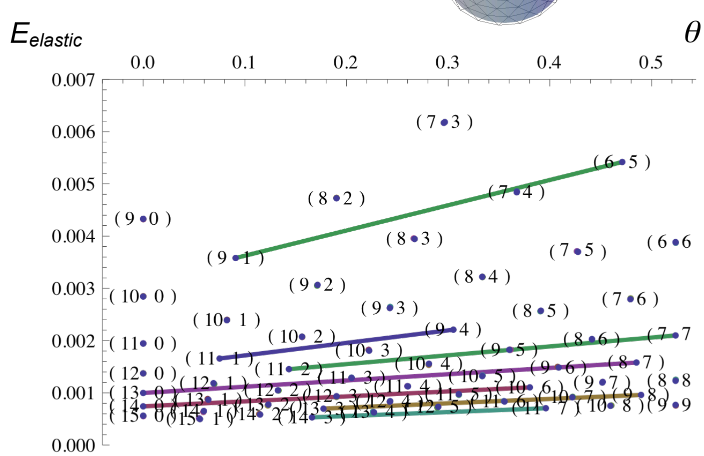




2:1 ionic lattice

3:1 ionic lattice





Armchair lattices

- Fibers tiled with *purely elastically interacting lattice* prefer armchair (*p, 0*) conformations (right plot)

(In both, the purely electrostatic and the purely elastic lattices, the lattice energies are plotted versus helical angle)