

A Model for Self-rolling of an Aluminosilicate Sheet into a Single Walled Imogolite Nanotube

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Since the discovery of carbon nanotubes and their inorganic counterpart, cylindrical structures have been intensely investigated by experimentalists and theorists. Imogolite is an attractive inorganic nanotube, present in weathered volcanic ashes [1]. It has found a variety of uses, among them as an effective arsenic retention agent [2], as a catalyst support, and as a constituent of nanowires. However, long after its successful synthesis, the details of the way it forms are not fully understood. By example, in Carbon Nanotubes, the graphitic sheet strain energy required to bend it into a Nanotube decreases monotonically, as the the nanotube diameter increases, thus precluding the possibility of tuning the NT diameter. With imogolite, on the contrary, highly monodisperse NT diameters are created.

Here we develop a viable model of the synthesis, which starts with a 2D planar aluminosilicate sheet as initial condition which is allowed to evolve freely, by means of classical molecular dynamics simulations, using the LAMMPS code [3]. For the interatomic interactions, the CLAYFF potential [4] is used, since it has been proven to be adequate to model aluminosilicate nanotubes. To optimize the nanotube structure and length of simulation cell to achieve better conformations, we used a combination of the minimization algorithm Fast Inertial Relaxation Engine (FIRE) and Conjugate Gradient (CG). In Fig 1. we show an schematic representation of the transition of the structure from 2D planar sheet to a minimal energy structure. The minimal structures that the system adopts are tubular, scrolled as well as more complex conformations, depending mainly on temperature as shown Fig 2. The minimal nanotubular configurations that we obtain are also strongly monodispersed in diameter, and quite similar in diameter to those of natural volcanic ashes, and to the ones that are synthesized in the laboratory. Moreover, a tendency towards nanotube agglomeration is observed, which is in agreement with experiments [5].

References

- [1] J. P. Gustafsson et. al. *Clays Clay Miner.* 49, (2001), 73.
- [2] N. Yoshinaga, et. al. *Soil Sci. Plant Nutr.* 8, (1962), 22.
- [3] S. Plimpton. *J. Comput. Phys.* 117, (1995), 1.
- [4] R. T. Cygan. *Phys. Chem. B.* 108, (2004), 1255.
- [5] V. C. Farmer et. al. *J. Chem. Soc., Chem. Commun.* 1977, 462.
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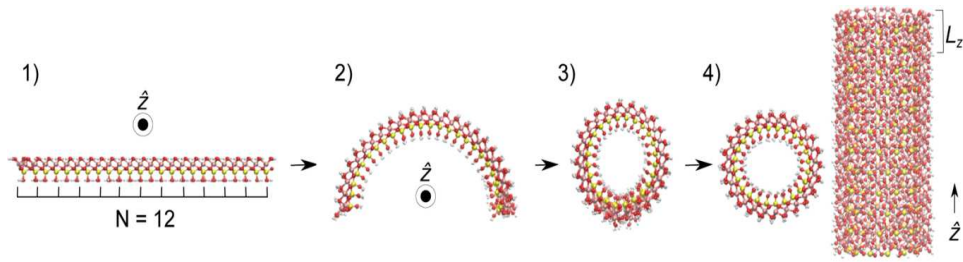


Figure 1: Schematic representation of the nanotube formation from 2D initial condition (1) to nanotube conformation (4).

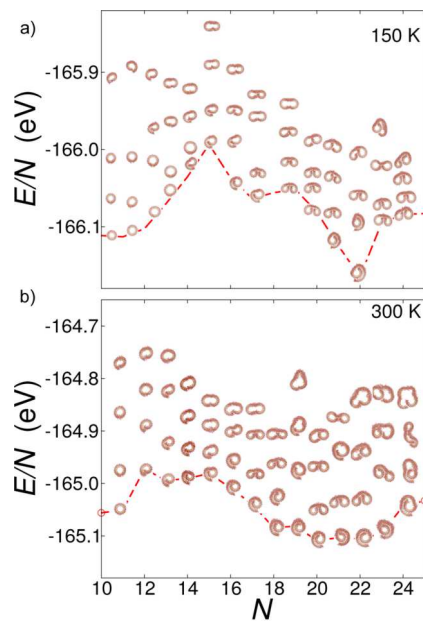


Fig 2: Families of conformations and of their energies, obtained from 2D initial conditions. The red line indicates the lowest energies for the various structures.