A Strategy to Model the Bending of 2D Materials

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Since 2004, when it was isolated for the first time, the unique two-dimensional (2D) lattice structure and physical properties of graphene have attracted much interest and excitement, mainly due to its extraordinary mechanical, electrical and thermal properties. For example, rippling of suspended graphene has been observed, with mesoscopic amplitudes and wavelengths. Also, supported monolayer graphene has been intensely studied. The effect of different metallic substrates has been investigated, showing that the rugosity can be tuned by varying the support. Recently, Zhou *et al.* reported on the interaction with a substrate where the graphene forms wrinkles and different conformations [1]. Theoretical studies have shown that the bending stiffness of the graphene monolayer is critical to achieve structural stability, and determines the morphology for both suspended and supported graphene sheets[2]. Moreover, it could have important effects on their electronic properties.

Other 2D materials similar to graphene, like h-BN, MoS_2 or WS_2 also have been the focus of attention, since control of the rugosity, or the use of wrinkles, favor some applications. Moreover, knowledge of the mechanisms to form different kinds of scrolled materials, is useful to confine others. The control of the stability, and the possibility to construct new heterostructures, is crucial to create models and to compare the mechanical properties of different structures.

The main objective of this work is to develop a strategy to calculate the bending energy of 2D materials. We use a soft external cylindrical force, specifically a Lennard-Jones (LJ) potential with an energy minimum equal to the curvature that is imposed. We apply this methodology to graphene, MoS_2 and Imogolite. The last one is a natural occurring aluminosilicate nanotube, that can be synthesized in the laboratory with well-controlled dimensions (both in length and radius).

References

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We first simulated the controlled bending of graphene using the LAMMPS code with energy optimizations (conjugate gradient and FIRE[3]). This way the sheet bends adopting the curvature imposed by the external LJ force. Next, we tested our strategy for the scrolling of MoS_2 and Imogolite sheets. The calculations were performed both classically and *ab initio*. For the first case we used the LAMMPS code[4], and for the latter we used density functional theory (DFT) as implemented in the VASP code[5]. These features are illustrated in Fig. 1 for graphene, MoS_2 and Imogolite.

In conclusion, we have developed a strategy to compute the bending energy of 2D materials, which can be applied to other 2D systems, which could be useful to develop continuous models for Imogolite, MoS_2 and graphene, with wrinkles and when rolling sheets are formed. They also may be helpful to predict mechanical properties of novel heterostructures. In addition, we calculated how finite size effects, due to the presence of border atoms, modify electronic and mechanical properties [6].

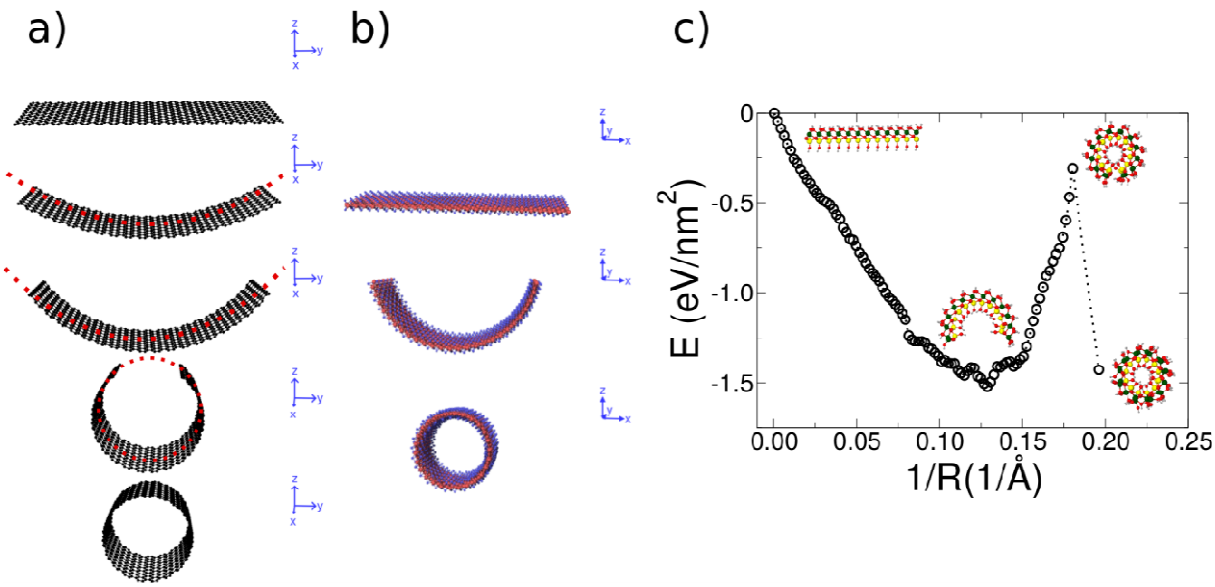

Figure 1: a) In red dashed lines we indicate the cylindrical Lennard-Jones force imposed to the 8 nm graphene sheet. Periodic boundary conditions along the cylinder axis. The energy of the system increases until the graphene sheet closes forming a CNT. b) MoS_2 bending. c) The special case of Imogolite nanotubes, where a minimun in the bending energy is found. The curvature is imposed to the Al atoms (black C; pink Mo; blue S; green Al; red O; yellow Si; light grey H).