AVVISO DI SEMINARIO

Giovedì 2 Luglio 2015 ore 14:30

nell'Aula Seminari del Dipartimento di Scienze e Tecnologie Chimiche, la

Dr. Emanuela Bianchi
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terrà un seminario dal titolo:

Anisotropy-driven assembly of nanoparticle model systems with directional interactions

Proponente: ***Dr. Federica Valentini***

Anisotropy-driven assembly of nanoparticle model systems with directional interactions

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Suitably designed coarse-grained models of particles at the nano-scale can provide a useful tool to investigate the collective behavior of a wide variety of systems, ranging from atomic/molecular to colloidal or polymer-based systems. Theoretical and simulation studies based of the assumption of spherically symmetric interactions between the constituent particles have led to tremendous advancements in material science. Nonetheless, the isotropy of the interactions is an idealization that can be treated as a zero-th order point of departure for the analysis of more complicated and realistic situations. Particles interacting

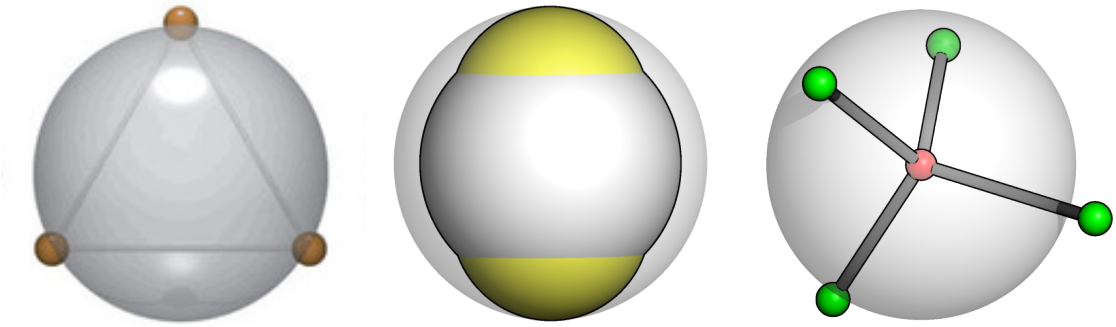

FIG. 1: Coarse-grained representations of: a conventional patchy unit with three bonding sites (left), an inverse patchy unit with two polar patches (middle), and a soft and flexible patchy unit with four attractive entities (right).

via anisotropic, directional and possibly selective potentials can model for instance water, silicon and carbon (at the molecular scale) as well as patchy particles (at the nano- and micro-scale). I will focus on three different classes of systems (see Fig. 1), namely (i) conventional patchy units [1, 2] – i.e. overall repulsive particles carrying a fixed number of attractive bonding sites in a pre-defined geometry –, (ii) inverse patchy colloids [3, 4] – i.e.

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patchy particles with charged surface regions –, and (iii) soft and flexible patchy units [5]– i.e. patchy particles with mobile patches–, and I will relate the features of these coarse-grained models to the physical systems underneath them. Subsequently, I will show some selected results about the equilibrium behavior of these systems, for instance the formation of open crystalline structures, such as the diamond and the honeycomb lattice, in the bulk as well as in two dimensions. Furthermore, I will introduce how a coarse-grained patchy model can be designed to reproduce desired features of graphene-like structures (see Fig. 2) and study, e.g., the behavior of defects in the honeycomb lattice.

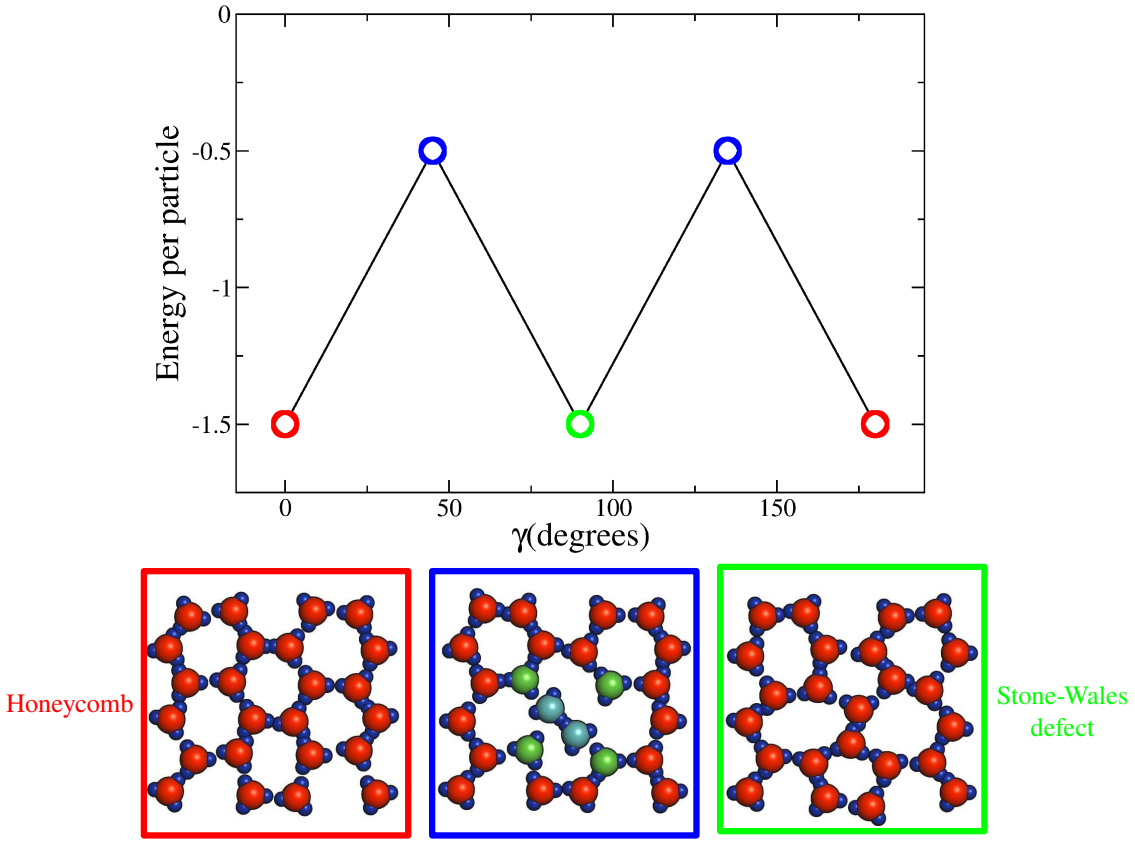

FIG. 2: Patchy model designed to reproduce the metastability of the Stone-Wales defect with respect to the honeycomb structure.

[1] E. Bianchi, J. Largo, P. Tartaglia, E. Zaccarelli and F. Sciortino, *Phys. Rev. Lett.*, 2006, **97**, 168301.

[2] E. Bianchi, R. Blaak and C. N. Likos, *Phys. Chem. Chem. Phys.*, 2011, **13**, 6397.

[3] E. Bianchi, C. N. Likos and G. Kahl, *NanoLetters*, 2014, **14**, 3412.

[4] E. G. Noya, I. Kolovos, G. Doppelbauer, G. Kahl and E. Bianchi, *Soft Matter*, 2014, **10**, 8464.

[5] E. Bianchi, B. Capone, G. Kahl and C. N. Likos, *Faraday Discussions*, 2015, DOI:10.1039/C4FD00271G.

Emanuela Bianchi received her Diploma (2005) and her PhD (2008) degrees in Physics from the University of Rome La Sapienza. Subsequently, she was at the Technical University in Vienna with an Erwin Schrödinger Fellowship in Mathematics and Mathematical Physics (2009), at the Heinrich Heine University in Düsseldorf as an Alexander von Humboldt fellow (2009-2010) and then back to the Technical University in Vienna first as a Lise Meitner fellow (2010-2012) and currently as an Elise Richter fellow (2012-present). Her work has been mainly focused on the equilibrium properties of systems characterized by directional effective interactions, with particular attention to collective behavior, such as gelation, phase separation, and cluster and crystal formation phenomena.