Annuncio di Seminario



Liquid crystals: device applications and computer simulations

Il seminario, aperto a studenti e docenti interessati, avrà luogo il giorno 10 novembre 2017 alle ore 12:00 nella sala affrescata del chiostro della Facoltà di Ingegneria di San Pietro in Vincoli in via Eudossiana, 18.

ABSTRACT. Liquid crystals (LC), with their unique combination of physical properties, continue to offer a number of novel fascinating applications ranging from optical and haptic displays to organic electronics devices, sensors, etc.. Microscopic models at various resolutions (lattice, molecular and atomistic) and their computer simulations provide important elements for the understanding of liquid crystal properties and the optimization of devices. In particular, atomistic molecular dynamics (MD) simulations can now make detailed and fairly reliable predictions of liquid crystal bulk properties. However, for most practical applications LC are not used in bulk but in micro or nano thick films where the LC is aligned with the help of surface interactions, so it is somewhat surprising that surface effects are still described only empirically, and that little is known on their molecular origin. Here we show that atomistic MD can shed some light also on the interfacial behavior of liquid crystals, e.g. in certain organic electronic devices. We also show examples for the prediction of the alignment and anchoring of LC (cyanobiphenyls in particular) at the interface with different solid surfaces e.g. silicon, crystalline and glassy silica with different roughness, soft self assembled monolayers and polymers.



BIOGRAPHY. Laurea from Univ. Bologna, IT,1972 (laude and M. Betti prize); PhD in Chemical Physics from Univ. Southampton, UK, 1975. Full Professor of Physical Chemistry at University of Bologna (1987-). Director of the International School of Liquid Crystals, Erice, IT (1998-). President of the International Liquid Crystal Society (2012-16). Chairman of European Supercomputing PRACE Access Panel (2012-2016). Invited Professor, Univ. Pavia (1998,2003,2010), Cambridge Univ., Newton Institute (Mar-Apr 2013); Univ. of Hyderabad, (2009-2010, 2012-2014), Univ. of Oxford, Mathematical Institute (Jan. 2014 and 2017), Univ. of Malaya, Kuala Lumpur (Aug 2015). Bonino medal of the Italian Chemical Society (2010). Research Topics: Atomistic, Lattice, Coarse Grain Computer Simulations, Theory and Spectroscopy of bulk and nano Liquid Crystals, Functional Materials for Organic Electronics applications, Proteins and other Soft Materials. Author of over 250 papers ((H=49 Google Scholar). Has given more than 300 invited lectures worldwide. He has supervised over 45 Master Thesis (Laurea), 19 PhD, and over 25 international predoctoral and 30 postdoctoral fellows (from BE, BR, CA, DE, FI, FR, GR, IN, IR, IT, JP, LT, NL, SE, SI, TR, UK). On the board of various international Journals, including Chem.Soc.Rev.,UK (2005-); MCLC, USA (1996-) ChemPhysChem, DE (2000-2014); PCCP, UK (1999-2002); J. Fluorescence, USA (1992-2001); J. Chem. Soc. Faraday Trans., UK(1993-1998); Molecular Physics, UK (1984-1992; 1998-2000); Liquid Crystals, UK (1986-1990).



