TIFR Centre for Interdisciplinary Sciences
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Seminar

Simulating the molecular organization of organic materials and its effects on charge transport

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Charge and energy transport in organic semiconductors, notably in those that present liquid crystal (LC) phases, are strongly affected by molecular organizations and their order, particularly close to relevant interfaces. Here we show some recent results for the computer simulation of these organizations at molecular and atomistic space resolution. With coarse grained, molecular level, models we can tackle, at least qualitatively, the effects that changes in the molecular structure have on the molecular organization. With atomistic molecular dynamics simulations we can now start to predict actual morphologies and physical properties at various temperatures and working conditions from a specific molecular structure and we present some applications to nematic and smectic liquid crystal systems and to some more specific organic electronics problems, e.g. organic solar cell design principles. We also tackle the problem of predicting alignment and anchoring strength of LC close to a solid interface, considering in detail thin films of 5CB on crystalline, hydrogen terminated silicon and on crystalline (cristobalite), amorphous silica surfaces of increasing roughness. In this last case we show that the crystalline surface enhances order at the interface, while the amorphous one reduces it. The importance of fabrication process, e.g. vapour deposition and annealing for the molecular organization close to a surface will be discussed.

Wednesday, Nov 26th 2014

4:00 PM (Tea/Coffee at 3:30 PM)

Seminar Hall, TCIS