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Hierarchical Modeling of Polymer/Solid Interfaces: From Ab-initio Calculations to Atomistic up to Coarse-grained Simulations VAGELIS HARMANDARIS, University of Crete, KAREN JOHNSTON, University of Strathclyde — We present a hierarchical simulation approach in order to study nanocomposite systems. Our approach combines quantum calculations, atomistic and coarse-grained (CG) dynamic simulations [1-2] and allows quantitative modeling of complex hybrid systems over a very broad range of length and time scales. As an example we model the polystyrene/gold system. The proposed scheme consists of the following stages: (1) Ab-initio (Density Functional Theory) calculations of a single molecule adsorbed on solid surfaces. (2) All-atom molecular dynamics simulations of short polymer chains/solid systems. We further develop a methodology to obtain rigorous CG models from the atomistic data, for specific polymer/solid systems. (3) CG simulations of more realistic polymer/solid surfaces. Structural, conformational and dynamical properties of systems with longer polymer chains are studied. The width of the interphase region of the polymer films found to be property specific, ranging from about 1.5nm to a distance that is proportional to the square root of the chain length. References [1] K. Johnston and V. Harmandaris, *J. Phys. Chem. C.*, **115**, (2011) 14707; *Soft Matter*, **8**, (2012) 6320. [2] K. Johnston and V. Harmandaris, *Macromolecules*, **2013,** *46*, 5741−5750.

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