Appunti di Fisica '18
&
Dottorato di Ricerca in Fisica

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Effective interactions in polymer nanocomposites

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Polymer composites containing nanosized particles are currently the object of a intensive investigation, for the capability of these material to generate new potential technologies [1]. In this context, the stability of the resulting nanocomposite material is of primary importance, since the addition of nanosized fillers into the polymer matrix can significantly influence its overall behavior. In particular, the potential of mean force (PMF) between the nanoparticles embedded in the polymer is the most investigated issue when studying the stability of polymer nanocomposites [2].

Here we present a simulation study of the PMF in a coarse-grained model of silica nanoparticles merged in a polystyrene matrix by using the hybrid particle-field molecular dynamics approach [3]. In our study, nanoparticles are considered both ungrafted and grafted with further polystyrene chains. The resulting interactions are strongly attractive if the nanoparticles are ungrafted, becoming progressively more repulsive upon increasing the grafting density. A deeper insight into the microscopic mechanisms underlying the effective interactions is gained by calculating the three-body contribution to the PMF; in such a way it is possible to compare our results with previous simulation [4] and experimental [5] morphological diagrams, finding a good correspondence between the behavior of the PMF and various self-assembled phases. In particular, it emerges that the knowledge of three-body effects is crucial for identifying the nature of self-assembled nanostructures, like strings, connected sheets or small clusters.

[1] C. Chevigny *et al, Macromolecules* 2011, **44**, 122.
[2] D. Meng *et al, Soft Matter* 2012, **8**, 5002.
[3] G. Milano and T. Kawakatsu, *J. Chem. Phys.* 2009, **130**, 214106.
[4] P. Akcora *et al, Nat. Mater.* 2009, **8**, 354.
[5] S. K. Kumar et al., *Macromolecules* 2013, **46**, 3199.

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