Dipartimento di Scienze Chimiche
Università di Napoli Federico II

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Aula CH2, ore 09.00

Host: Prof. Nadia Rega

Simulating biological systems coupling particles and fields with molecular dynamics

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The hybrid particle-field with molecular dynamics (hPF-MD) is a newly-established methodology based on density-functional potentials for the simulations of molecular systems [1]. Thanks to its low computational costs, hPF-MD is capable of treating large-scale soft matter systems using relatively small high-performance architectures [2]. As case examples, I will first present the first hPF-MD model for peptides, showing how it is able to sculpt the main features of the folding diagram for model hydrophobic-polar sequences [3]. Then, I will introduce advances in the fundamental electrostatic theory for density-field in both homogeneous and non-homogeneous dielectric [4]. This is a crucial ingredient to expand the application range of hPF-MD to generalised biological systems, which are characterized by a strong polar/ionic character. I will show how they can be effectively used to simulate polyelectrolytic systems like charged surfactants or polar-apolar mixtures [5].

References

[1] G. Milano and T. Kawakatsu, J. Chem. Phys. 130, 214106 (2009).
[2] T. Soares, S. Vanni, G. Milano, and M. Cascella, J. Phys. Chem. Lett. 8, 3586 (2017).
[3] S. L. Bore, G. Milano, and M. Cascella, J. Chem. Theory Comput. 14, 1120 (2018).
[4] S. L. Bore, H. B. Kolli, T. Kawakatsu, G. Milano, and M. Cascella, submitted.
[5] H. B. Kolli et al., J. Chem. Theory Comput. 14, 4928 (2018).