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 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 dielectrics [4]. This is a crucial ingredient to expand the application range of hPF-MD to a large variety of biological systems, which are characterized by a strong polar/ionic character.

References

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