



سمینار هفتگی ماده چگال نرم

****لطفاً به زمان نامتعارف سمینار توجه فرمایید****

Particle-Based Simulation Methods in Computational Materials Chemistry; few case studies from gas phase to solid state

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Abstract

An improved understanding of the matter at the nanoscale will yield novel insights in diverse fields such as physics, chemistry, biology, materials science, and environmental science. Theoretical and computational modeling has significantly advanced our understanding of a wide variety of nanoscale phenomena. Anchored by comparisons to experimental data, carefully designed computational models can provide key mechanistic insights that often, as a result of physical limitations, elude experimental design. In this presentation, I will review some of my recent works in studying gas phase chemical reactions, interfacial structure and heat transfer in polymer nanocomposites, laser ablation in 2D materials, as well as thermoresponsive behavior of metal organic frameworks.

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