Molecular interactions to material properties: computational methods to bridge the scales

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Understanding the interplay of molecular interactions that govern the self-assembly and material properties of biological and soft matter systems remains a challenging task for experiment and theory. Small changes at atomistic scale modulate the mechanical and dynamic properties of molecular assemblies such as lipid bilayers or protein aggregates, at much larger length and time scales. These different scales make it difficult to understand these systems as a whole.
While molecular dynamics (MD) simulations at the atomistic level contain a lot of chemical details they are limited to small molecules and nanosecond timescales. More coarse-grained methods on the other hand, can access much greater length and timescales, but lack chemical detail and often require the determination of many free parameters.
This talk will give examples for the uses of both approaches, and introduce procedures for the development of hierarchical models, which build on the information from the atomistic scale to systematically obtain more coarse-grained representations.