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Soft Matter Properties: What can we learn from computer simulations?

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<p>I will present three unrelated examples in which efficient computer simulations have been employed to address soft matter properties. The first example will deal with the dynamics of polymers near surfaces. Despite the significant progress within the last decade, in particular on the structure and thermodynamic properties in confinement, their dynamics remained an active field of research. Unlike some of the prior studies, we introduced atomic scale roughness of the confining surface(s) while abstaining from introducing any artificially-imposed divergent obstacles. Because of this type of modeling, we could reproduce the scaling of the single polymer dynamics near attractive surface and relate the dynamics of adsorbed polymer films with the degree with which they interlock with the surface. The second example will explore the mechanical behavior of highly cross-linked polymer (HCP) glasses; such as epoxy and vinyl-ester thermosets, which are used as both high-strength adhesives and as composite matrices. One particular property of HCPs which limits their usefulness is their lack of toughness. Fully cured epoxies, for example, can have about 2 GPa of tensile strength but are brittle, failing at about 1

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