Structure and dynamics of Curcumin-Vacuum and Curcumin-supercritical CO_2 interfaces: A molecular dynamics analysis

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Controlling the polymorphic forms of active pharmaceutical ingredients (APIs) is a major challenge for both basic research and the pharmaceutical industry. Recent advances have highlighted the crucial role played by the surface properties of different crystalline structures, and in particular by the conformational distribution of API molecules at the solid interface, in promoting polymorphism.

In this context, this talk presents an in-depth study of the interface between curcumin (CUR) and supercritical carbon dioxide ($scCO_2$) using molecular dynamics (MD) simulations. Curcumin, a molecule subject to growing interest in medicine, has been parametrized, based on quantum chemical (QC) calculations, in order to accurately reproduce thermodynamic differences between its three polymorphs as well as their corresponding conformational distributions of CUR molecules.

We have developed new algorithms for sampling CUR conformations, as well as for calculating various structural and dynamic properties at its interface. In order to reliably study the CUR-$scCO_2$ system, we have evaluated several force fields for the CO_2 and identified the one that most faithfully reproduces the critical point properties. We demonstrated how certain local observables can be used to characterize the organization and dynamics of the supercritical fluid near the critical point. This protocol was then applied to compare the structural and dynamic behaviors of $scCO_2$ with those of water and ammonia in their respective supercritical regimes.

Finally, we characterized local structural changes at the CUR-vacuum and CUR-$scCO_2$ interface under different thermodynamic conditions. A specific algorithm was used to identify the CUR molecules belonging to each interfacial layer, allowing a fine analysis of the structural, dynamic and energetic properties within these critical regions for the stability and evolution of polymorphic forms.