Project Title: Molecular modeling of organic matter – clay mineral interactions and its application on the study of surface-enhanced nucleation and clathrate hydrate formation.

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Project Abstract:

Clay minerals have always had a special place in the study of surface and interface effects, which have applications ranging from sorption of heavy metals to clathrate hydrate formation. In recent years, a resurgence of environmental awareness has prompted for the advancement of research on the mitigation of greenhouse gases through hydrate-based encapsulation technologies using mineral-rich natural storage sites (e.g. geologic or subsea), but the task of understanding the feasibility of the processes involved is hampered by the formulation of models by which thermodynamics properties may be predicted over appropriate space and time scales. By itself, aqueous solutions of greenhouse gases, such as CO$_2$, can be controlled through pressure and temperature variations to achieve incipient clathrate formation. Mineral surfaces appear to promote hydrate formation by providing well ordered lattice sites for nucleation. Earlier studies also indicate the role of organic matter on the promotion of hydration formation. While much knowledge has been gained on the bulk, structural, and molecular properties of clay minerals, the molecular mechanisms that govern surface kinetics of different processes that can occur on clay mineral surfaces, however, are still left as open questions.

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