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Thermodynamics of Materials and Minerals under Confinement: From Ionic and Organic Solids to Refractory Ceramics

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Nano and subnano-scale confinement phenomena govern both geochemical and engineering processes, ranging from the transport of nutrients, and contaminants in minerals near the earth's critical zone, to heterogeneous catalysis, separation, and energy storage in synthetic materials for a more sustainable future. This talk summarizes our studies on the thermodynamics of materials under 2D and 3D confinement or encapsulation during the past 7 years. The systems presented include (i) layered double hydroxides (LDHs) in iodine separation and capacitive energy storage, (ii) interfacial and structural heterogeneity of MXenes synthesized under CoF_x/HCl etching environment, and (iii) design of stable transition metal oxide/carbide - zeolite catalysts for hydrogen production and methane conversion. In all these systems, thermodynamics plays a critical role in paying for the energetic costs of the metastable guest species and defective interfaces, and in the determination of nanoscale molecular structures at the interfaces and macroscale material functionalities in applications.