Energetics of the oil interaction with calcite and kerogen – Implications for hydrocarbon transport and storage in shale

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Characterizing the behavior of oil molecules in nanopore is vital to the understanding of geochemistry of hydrocarbon-bearing fluid in ultra-tight source rocks, such as shale. The heterogeneous nature of hydrocarbon system of nanoscale complicates experimental studies of oil / shale interfacial interactions. Therefore, to understand the mechanism of the interplay of oil molecules in rock nanopore, we applied molecular dynamics simulations to study the interactions of polar and non-polar oil on both calcite and kerogen surfaces with and without water. The effect of surface wetting, oil polarity, and temperature on the Gibbs free energy surface of adsorption are investigated. The interaction free energy, entropy, and enthalpy are calculated using advanced molecular dynamics method - umbrella sampling. In agreement with current understanding based on experimental studies, our results show that: 1) surface with adsorbed water layer significantly reduces the oil adsorption energy on kerogen and turns the calcite surface to highly oil-repellent; 2) polar oil has overall stronger adsorption free energy than that of non-polar oil on both non-wetted calcite and kerogen surfaces; 3) organic surface (e.g. kerogen) exhibits stronger adsorption of oil molecules compared to inorganic one (e.g. calcite). The finding of this study indicates that oil displacement in nanopores can be enhanced by promoting the water adsorption on surface and reducing the polarity of oil on both inorganic and organic interfaces.