Multi-scale models of kerogen in gas shales

R. Vermorel[1], A. Botan[1], L. Brochard[1], G. Hantal[1] and R.J-M Pellenq[1]

[1]*Massachusetts Institute of Technology, Cambridge, MA, USA*

ABSTRACT: Over the past decade, petroleum industry's interests have increasingly focused on natural gas production from gas shales. These unconventional reservoir rocks exhibit a singular microstructure, which consists in a mixture of inorganic mineral grains and nanoporous organic patches, the so-called "kerogen". The term kerogen refers to a broad variety of sedimentary organic materials, which have maturated under geological confinement conditions[2]. In the final stages of the maturation process this organic matter can be viewed as a porous carbon skeleton containing adsorbed oil and gas. How the mechanical and transport properties of gas shales relate to the molecular structure of kerogen is still an open question. In this work, we propose an approach based on the Hybrid Reverse Monte Carlo method[3] to reconstruct an atomistic model of kerogen consistent with experimental data. This molecular model is used to study the adsorption and transport properties of the nanoporous kerogen at small scales. In addition, we have devised a coarse grained polymer-like molecular model to study the mechanical properties of kerogen at larger scales. First results and comparison with experimental data are reported.

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[3]*S.K. Jain et al., Langmuir 22 (2006) 9942-9948*