Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A6]Symposium A-6

Chair: Emma Griffiths(University of Cape Town, South Africa)
Wed. Oct 31, 2018 11:15 AM - 12:30 PM Room6

[SY-A6]From cellulose and lignin to kerogen: molecular simulations of a geological process

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The process by which organic matter decomposes deep underground to form petroleum and its underlying kerogen matrix has so far remained a no man’s land to theoreticians, largely because of the geological (Millions of years) timescale associated with the process. Using a replica exchange accelerated molecular dynamics method initially developed in the context of the micro- to milli-second timescale for protein folding, we simulate the full transformation of cellulose and lignin (the main components of wood) into kerogen under prevailing geological conditions. We observe in sequence (i) the fragmentation of the cellulose crystal and production of water, (ii) the development of an aliphatic macromolecular phase, (iii) its aromatization, and (iv) its aggregation into a stiff porous aromatic carbon upon expulsion of the fluid phase. The composition of the solid residue along the maturation pathway strictly follows what is observed for natural type III kerogens and for artificially matured samples under closed conditions, providing further evidence of a kinetically controlled, irreversible, decomposition process in which the aliphatic (immature) phase is a metastable intermediate.