NEW OPPORTUNITIES IN THE APPLICATION OF THE ClayFF FORCE FIELD FOR ATOMISTIC COMPUTER MODELING OF NATURAL AND SYNTHETIC NANOPOROUS MATERIALS AND THEIR HYDRATED INTERFACES

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Molecular-level knowledge of the thermodynamic, structural, and transport properties of water and aqueous solutions confined in nanopores and at interfaces with clays, cement, and other natural and synthetic inorganic nanomaterials is crucial for quantitative understanding and prediction of many technological and environmental processes, including rock weathering, geological nuclear waste storage, water desalination, geological carbon sequestration, etc. Atomistic computational modeling is capable to significantly complement the experimental investigations of such systems by providing invaluable atomic-scale picture of the materials and processes involved, leading to a greatly improved understanding of the specific effects of the substrate structure and composition on the structure, dynamics and reactivity of the interfacial and nano-confined aqueous solutions. However, accurate and realistic molecular scale simulations of such materials as clays are often challenging, because of the great diversity of their chemical composition the significant degree of their structural and compositional disorder. ClayFF was originally developed in response to a strong need for a robust and flexible force field for classical atomistic simulations of such materials and interfaces, as well as their interactions with organic and bio- molecules in aqueous environment [1]. This lecture will provide a brief overview of the fundamental assumptions and limitations of the ClayFF approach to the atomistic modeling of these complex systems and demonstrate new opportunities offered by recent improvements of ClayFF, specifically addressing the simulation of a wide range of materials related primarily to clay and cement chemistry [2-4]. [1] R.T. Cygan, J.-J. Liang, A.G. Kalinichev (2004) J. Phys. Chem. B, 108, 1255-1266. [2] M.Szczerba, A.G.Kalinichev (2016) Clays Clay Min., 64, 488-502. [3] I. Androniuk, C. Landesman, P. Henocq, A.G. Kalinichev (2017) Physics and Chemistry of the Earth A/B/C, 99, 194-203. [4] M.Pouvreau, J.A.Greathouse, R.T.Cygan, A.G.Kalinichev (2017) J. Phys. Chem. C., 121, 14757-14771.