Department of Chemistry and Biochemistry
Physical Chemistry Seminar Series

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Monday, February 25, 2019 ~ 2:00 pm 331 Klamath Hall

Multiscale modeling of polymer controlled crystallization of calcium oxalate from solution

Crystallization of calcium rich minerals, such as calcium carbonate, calcium oxalate and hydroxyapatite, affects several forms of life, from plants and animals to human beings. These minerals are fundamental constituents of shells and bones, but are also associated to pathology. Understanding and controlling crystallization of these materials at a molecular level in biological environment would allow medical scientists to design countermeasures to prevent common diseases, such as urinary tract stones and hydroxyapatite crystal deposition. Mineralization in solution, assisted or inhibited by electrolytes, is a process that entails a broad range of size and time scales. To gain molecular insight by computer simulations thus requires carefully designed multiscale modeling techniques, and data analysis tools.

Here we consider the case of calcium oxalate, the main component of kidney stones, and we investigate its nucleation and growth in aqueous solution, in the presence of polypeptides, e.g. poly-glutamate, that have been shown to slow down nucleation, and to select mineral structure and morphology. With a combination of classical and ab initio molecular dynamics, and advanced sampling techniques, we unravel the interaction of poly-glutamate with ions in solution and at the surface of crystalline calcium oxalate. Furthermore, we introduce a Hamiltonian adaptive resolution scheme (H-AdResS), which allows one to concurrently treat a liquid system at different levels of details at controlled thermodynamic conditions, thus making it possible to simulate directly the nucleation and growth of minerals in solution.

Refreshments served at 1:45 pm 331 Klamath Hall

Hosted by Marina Guenza