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Mechanisms of Molecular Recognition & Assembly at the Nanoscale: Computation Meets Experiment

Tuesday, March 17

90 Snell Library
11:15am – 12:30pm

*Refreshments will be
served*

ABSTRACT The complexity of the molecular recognition and assembly of biological and nanostructured interfaces on a scale of 1 to 1000 nm can be understood more effectively using simulation tools along with laboratory instrumentation. Examples of biomolecule recognition on nanostructured metals, silica, and apatites illustrate insight into molecular recognition mechanisms in 3D atomic resolution towards improving catalysts, sensors, and therapeutics. The adsorption mechanism of peptides on metal surfaces was discovered computationally to involve coordination of polarizable atoms in the peptide (C, N, O) with epitaxial sites on the metal surface, as well as contributions from induced charges. Computation predicts facet-specificity and preferred nanoparticle shape in correlation with laboratory synthesis, X-ray, TEM, and spectroscopy, as well as catalytic reactivity using reactive extensions of the force fields. For oxidic minerals such as silica, the explicit consideration of the surface chemistry as a function of pH and particle size allows quantitative predictions of peptide adsorption, including sensitive point mutations. Similarly, the nanostructure of hydroxyapatite and its major facets varies strongly with pH, showing very different surface definition and binding mechanisms of proteins and osteoporosis drugs. A key development in our team has been the INTERFACE force field which unites materials and biomolecular simulation in a single platform and improves the accuracy of prediction of interfacial properties up to two orders of magnitude. A wealth of information in atomic resolution and at the

mesoscale is becoming accessible by such computer-aided models in partnership with synthesis, processing, and characterization efforts to accelerate materials discovery.

BIOGRAPHY Hendrik Heinz earned his Diploma (M. S. degree) in Chemistry and his doctorate in Materials Science and Engineering (2003) at ETH Zurich, and then carried out postdoctoral work at the Air Force Research Laboratory at Wright-Patterson Air Force Base, Ohio. Subsequently, he joined the world's largest polymer research program in the College of Polymer Science and Polymer Engineering at University of Akron in 2006 where he is currently an associate professor. His research interests include multi-scale simulation of biomaterials, organic-inorganic composites, minerals, catalysts, as well as the development of computational methods, particularly accurate force fields for numerous metals and oxides. He established the first uniform simulation platform for inorganic-organic and inorganic-biological interfaces at the 1 to 100 nm scale consistent with existing force fields for biopolymers and organic compounds. He has been an invited guest professor at NIMS/MANA (Japan) as well as at ETH Zurich. Awards include the 2013 Max Hey Medal of the Mineralogical Society (UK), the George Brown Lectureship at Euroclay 2011, an NSF Career Award, the Giovanni Novelli Prize of the Italian Clay Group, as well as an HP Outstanding Junior Faculty Award from ACS.

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