THE MATERIALS SCIENCE AND ENGINEERING DEPARTMENT SPRING COLLOQUIUM SERIES PRESENTS:

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## Peptide surfactants for lanthanide recovery

Rare earth elements (REEs), crucial to modern technologies, are notoriously difficult to separate from each other owing to the similar diameters of the REE cations and the fact that they are typically present in th (+3) oxidation state. We are developing an environmentally friendly REE separation process which exploits peptide surfactants (PEPS) inspired by biology that bind selectively to REEs and bring them to the air-water interface for recovery via a froth flotation process. The success of this approach requires that the PEPS ability to bind selectively to REE cations is retained in the highly anisotropic environment of the fluid interface. Researchers drawn from the University of Pennsylvania, the City College of New York, the University of Illinois at Chicago and Northwestern University have teamed to advance this vision. I share highlights of our current state of understanding, insights gleaned into PEPS:REE cation complex behavior in the fluid interface, and our current challenges.

As an initial PEPS structure, we have studied a known surface-active lanthanide binding tag peptide designed to coordinate via multidentate interactions with REE cations in a binding loop inspired by the highly conserved EF-hand binding sequence in calcium binding proteins. The concentration of PEPS and cations adsorbed at the interface, characterized by X-ray reflectivity and X-ray fluorescence near total reflection methods at NSF's ChemMatCARS facility, indicate that more cations than peptides are present in the interfacial layer when equimolar or greater concentrations of cations to peptides are present in solution. This is an undesired outcome. We hypothesize that REE cations have two modes of interaction with the PEPS; interaction via the selective binding loop and via non-selective Coulombic interaction owing to net charge on the PEPS:REE complex. To eliminate excess adsorbed cation, peptide mutants designed to form PEPS:REE complexes with reduced the net charge are studied via X-ray characterization methods, confocal imaging, and surface rheology, informed by metadynamic and molecular dynamics simulations. The results suggest that the PEPS binding loop remains intact in the air-aqueous interface, and that nonspecific Coulombic interactions with REE in solution can be avoided, essential features to our envisioned process. Ongoing work focuses on understanding the differences in in PEPS selectivity among REE cations in bulk solution and at the interface.

**Kathleen J. Stebe** is the Goodwin Professor in the School Engineering and Applied Sciences at the University of Pennsylvania. Educated at the City College of New York, she received a B.A. in Economics and a Ph.D. in Chemical Engineering at the Levich Institute advised by Charles Maldarelli. After a post-doctoral year in Compiegne, France under the guidance of Dominique Barthes-Biesel, she joined the Department of Chemical Engineering at Johns Hopkins University, where she became Professor and served as the department chair. Thereafter, she joined the University of Pennsylvania, where she served in various administrative capacities including department chair and Deputy Dean. She has been recognized by the National Academy of Engineering, the American Academy of Arts and Sciences, the Johns Hopkins Society of Scholars, and as a Fellow of the American Physical Society and of the Radcliffe Institute. Her research focuses on directed assembly in soft matter and at fluid interfaces, with an emphasis on confinement, geometry, and emergent structures in far from equilibrium settings for novel functional materials.

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In person only; no Zoom Questions? Contact <u>allison.macknick@northwestern.edu</u> and megan.ray@northwestern.edu