PHYSICAL CHEMISTRY SEMINAR

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"Tailoring Functionalized Interfaces for Advanced Energy Applications"

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ABSTRACT:

Interfaces are crucial in determining the performance of a broad range of materials used in energy-critical applications. Scientific challenges underlying transformative technologies for energy storage, quantum computing, and chemical separations may be addressed by preparing well-defined functionalized interfaces amenable to detailed experimental characterization and theoretical modeling. Our team is focused on establishing the fundamental scientific understanding and structure-function relationships necessary to enable the predictive design of nanoengineered interfaces for various energy-related tasks. In short-term energy storage, sub-nanometer-sized metal oxides known as polyoxometalates have been investigated as leading candidates for supercapacitors. We demonstrate how the surface morphology, redox properties, and charge storage capacity of supported polyoxometalates evolve with atom-by-atom substitution in the presence of differently functionalized surfaces and how these properties may be tailored to optimize energy storage performance. In materials for quantum computing, polyoxometalate-based molecular qubits doped with electron spin elements have been demonstrated as promising alternatives to traditional solid-state qubits. We establish how the vibrational properties of supported polyoxometalate qubit arrays, which determine their practical spin decoherence rates for quantum computing, are influenced by specific qubit-qubit and qubit-substrate interactions. In chemical separations, spatially confining environments, tailored electrode-electrolyte interfaces, and externally applied electric and magnetic fields have been identified as promising means of achieving the efficient and selective extraction of metal ions from aqueous feedstocks. We illustrate controlled and reversible metal ion binding in the confined interlayer transport channels of functionalized graphene oxide membranes. We also demonstrate increased water flux through the restricted nanoscale channels of membranes by functionalizing graphene oxide with hydrophobic ionic liquids. At electrode-electrolyte interfaces, we establish how the properties of ionic liquid clusters influence their efficiency toward the adsorption of targeted ions by introducing hydrophobic domains that lower the overpotentials for metal reduction. The fundamental understanding of functionalized interfaces obtained from our research informs the design of improved materials for advanced energy storage technologies, quantum computing applications, and the extraction of the critical materials needed to power our nation's clean energy revolution.

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