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Festschrift for Judith Herzfeld: spectroscopic and theoretical studies of biomolecules, aqueous solutions, and materials

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The themed collection 'Festschrift for Judith Herzfeld: spectroscopic and theoretical studies of biomolecules, aqueous solutions, and materials' brings together a broad range of experimental and theoretical studies, including quantum mechanical and semi-empirical computations of water, protein dynamics, and action mechanisms of membrane transporters and receptors that use retinal to trigger reactions. Papers from the themed issue discuss state-of-the-art methodological developments in computation and experiment, and their applications to understanding fundamental physical–chemical principles of biological systems and materials.

The themed collection opens with two articles by Prof. Herzfeld, a retrospective (https://doi.org/10.1039/d4cp90021a) and a reflection on the cross-talk between experiment and theory (https://doi.org/10.1039/d4cp00005f). In 1972 Prof. Herzfeld obtained her PhD in chemical physics from MIT where, together with H. E. Stanley, she developed a general model for co-operativity in hemoglobin; half a century later, their paper[1] is still cited. In 1973 Prof. Herzfeld started her independent academic career as a tenure-track assistant professor of chemistry at Amherst College, then moved to the Harvard Medical School, where she first joined the Biophysical Laboratory and then the Department of Physiology and Biophysics. While at the Biophysical Laboratory Prof. Herzfeld published, with A. E. Berger, a highly influential paper titled "Sideband intensities in NMR spectra of samples spinning at the magic angle".[2] In 1985 Prof. Herzfeld joined the Department of Chemistry at Brandeis University, where she developed a research program that brought seminal contributions to the fields of NMR spectroscopy, statistical thermodynamics, and chemical education. Most recently, Prof. Herzfeld developed semi-classical approaches for efficient computations of molecular structures[3,4] and simulations of chemical reactions.

This topical collection, celebrating the research achievements of Prof. Herzfeld, includes papers by colleagues and collaborators. Naturally, the research topics covered by the issue are broad.

Many of the contributions to this themed collection use NMR or FTIR spectroscopy to investigate the structure and dynamics of biomolecules, biomolecular complexes, and complex mixtures. Vugmeyster and colleagues (https://doi.org/10.1039/d3cp04824a) and Golota and colleagues (https://doi.org/10.1039/d4cp00553h) rely on NMR spectroscopy to characterize the structure and dynamics of amyloid-beta fibrils. A combination of solution and solid-state NMR with atomic force microscopy and fluorescence assays is used by Sridharan and colleagues (https://doi.org/10.1039/d4cp03593c) to show that binding of copper ions alters the conformation of prion protein amyloid fibrils. Richard and colleagues (https://doi.org/10.1039/d4cp01268b) present the ^{13}C NMR assignments for cytochrome P450 CYP17A1 bound to a cancer drug, whereas Pankratova and colleagues (https://doi.org/10.1039/d4cp01648c) use solid-state NMR to identify protonation states of amino acids and the protonation-coupled dynamics of a viral proton channel. Zhang and colleagues (https://doi.org/10.1039/d3cp06280e) present a new method that allows for background signal to be suppressed in dynamic nuclear polarization (DNP) NMR spectroscopy of complex mixtures. Dsouza and colleagues (https://doi.org/10.1039/d4cp00221k) combine magic angle spinning (MAS) NMR with other spectroscopic and structural biology approaches to characterize chlorosomes.

Two of the contributions to this themed collection focus on microbial rhodopsins, *i.e.*, proteins from the same family as the bacteriorhodopsin proton pump studied by Prof. Herzfeld. Using

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low-temperature FTIR spectroscopy, Nishikino and colleagues (**https://doi.org/10.1039/d4cp02248c**) demonstrate the key role of the color-switching residue for the absorption maxima of the green- and blue-absorbing proteorhodopsins. Pinto and colleagues (**https://doi.org/10.1039/d4cp02611j**) report on solid-state NMR data and hydrogen-bond network analyses that identify the local hydration pattern as a key determinant of the direction of proton pumping in microbial rhodopsins.

To evaluate how certain conformational transitions of a bacterial repeat-in-toxin protein are influenced by the addition of a polymer, Chenal & Minton (**https://doi.org/10.1039/d4cp02213k**) develop a unified excluded volume model that makes use of the effective hard particle approximation. The paper by Berger (**https://doi.org/10.1039/d4cp02217c**) studies the conditions under which an iterative procedure to compute a cylindrically symmetric orientation distribution function for rod-like particles converges. The energetic analysis developed by Finkelstein and colleagues (**https://doi.org/10.1039/d4cp00818a**) allows the authors to explain how discharging lithium-ion batteries work.

Systematic studies of relevant model systems and proofs-of-concepts for the applicability of computational approaches are valuable references for physical chemistry. In this topical collection, Sun and colleagues (**https://doi.org/10.1039/d4cp01393j**) demonstrate that semi-empirical methods provide a reasonable description of charge transfer in metal nanocluster dimers that would otherwise be difficult to study with TDDFT; Stevens and Rempe (**https://doi.org/10.1039/d3cp04200f**) apply DFT to characterize the lowest binding free energies and structures of model carboxylate–water–cation complexes relevant to ion binding in biology.

We anticipate that this topical collection celebrating the research of Prof. Judith Herzfeld will remain as a reference for its compelling view of modern experimental and theoretical approaches to fundamental aspects in physical chemistry and chemical physics.

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