Department of Chemistry Seminar Series
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Switchable host-guest interactions of cationic macrocycles

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Intermolecular forces and shape complementarity control binding interactions found in molecular systems such as enzyme-substrate complexes. Taking inspiration from nature, organic chemists have built a plethora of host-guest systems, and used them for various applications, from highly selective and sensitive chemical sensors to molecular machines that can perform unidirectional motion. In this talk, I will discuss two different projects involving polycationic molecular hosts, focusing on the modulation of host-guest interactions using different inputs. 1) Redox and acid–base chemistry are well-established stimuli to switch supramolecular systems. I will introduce a cationic macrocycle that can be switched by either of these two pathways, resulting in clear changes in affinity towards different polycyclic aromatic compounds (PAC). 2) Host-guest binding can be influenced by the presence of competitor binders. I will discuss how we are using this competitive binding for growing diffraction quality single crystals of highly insoluble PACs. Throughout this talk, I will explain how we use analytical tools such as NMR spectroscopy and X-ray crystallography to elucidate these complex systems.