From Frameworks to Cages: Computational Strategies for Complex Molecular Architectures

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The discovery of new materials drives societal progress, from the Bronze and Iron Ages, to the current era of advanced functional materials. Due to the combinatorial explosion of materials choice, modern scientific and technological challenges require the coexistence and integration of a diverse ecosystem of materials types and classes. This widened design space necessitates solutions beyond brute force, searching for the "need in a haystack" on trial and error intuition alone is cumbersome and expensive. Computational sciences bring an umbrella of algorithms and models, but the challenge remains: how can we merge chemist intuition with the scale and efficiency of computational chemistry?

In this lecture, I will discuss the recent advances in computational chemistry for materials discovery, with a particular emphasis on designing low-symmetry supramolecular systems. By combining high throughput computational screening with evolutionary algorithm approaches, we can efficiently navigate vast regions of chemical space, therefore enabling the design and optimisation of materials with tailored functions. Beyond specific targets, screening thousands of experimentally validated and hypothetical structures (e. g. metal organic frameworks) has the potential to reveal generalisable design rules, further guiding experimental efforts towards the most promising regions of chemical space.

I will highlight our recent efforts in discovery of low symmetry supramolecular materials, showcasing how predictive modelling and algorithmic design can uncover emergent structural motifs, opening new avenues for supramolecular materials chemistry. The lecture will continue with a broader discussion on the role of interdisciplinary dialogue between theory and experiment in shaping the future of molecular sciences.

References

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