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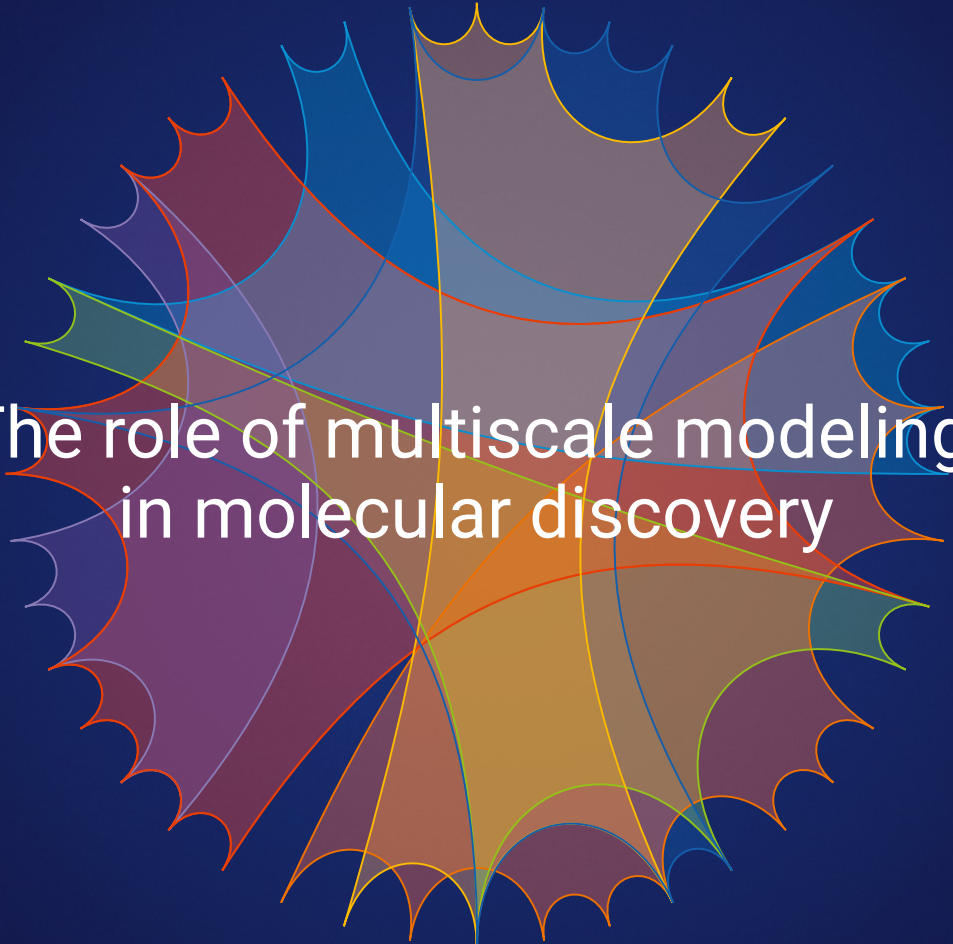


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STRUCTURES JOUR FIXE

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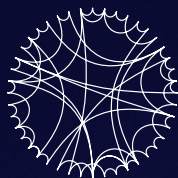
The role of multiscale modeling
in molecular discovery

July 07, 2023, 1:30 PM, Phil 12 GHs

COFFEE & SNACKS IN ROOM 106

ZOOM: Meeting ID: 935 6549 3662, Code: 928036

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ABSTRACT

Advanced statistical methods are rapidly impregnating many scientific fields, offering new perspectives on long-standing problems. In materials science, data-driven methods are already bearing fruit in various disciplines, such as hard condensed matter or inorganic chemistry, while comparatively little has happened in soft matter. I will describe how we use multiscale simulations to leverage data-driven methods in soft matter. We aim at establishing structure-property relationships for complex thermodynamic processes across the chemical space of small molecules. Akin to screening experiments, we devise a high-throughput coarse-grained simulation framework. Coarse-graining is an appealing screening strategy for two main reasons: it significantly reduces the size of chemical space and it can suggest a low-dimensional representation of the structure-property relationship. I will briefly mention a biological application of our methodology that led to the discovery of *in vivo* active compounds. Finally, I will mention a number of ways machine learning can help fulfill the promise of connecting models at different scales.

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