Institute of Science and Technology Austria

SLAM Seminar

Catalysis from the bottom-up: towards artificial catalytic matter

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Host: Andela Saric

Catalysis, the acceleration of chemical reactions by molecules catalysts that are not consumed in the reaction, is central to living organisms. Indeed, living organisms rely on enzymes, natures unparalleled catalysts, to regulate metabolic and signaling pathways with high specificity and remarkable catalytic activity. Despite their ubiquity in both biology and chemistry, elucidating the general design principles of efficient catalysts remains a major challenge, with artificial enzymes failing to meet the capabilities of their natural counterparts. In particular, there is no theoretical framework to rationally build catalysts from scratch. To address this challenge, we propose a model to study and design catalysis from the bottom-up using a coarse-grained system of building blocks interacting via programmable potentials. We define catalysis as a first passage process and focus on accelerating a fundamental reaction, the cleavage of a bond, with a minimal catalyst architecture, a rigid dimer. By combining theory and molecular dynamics simulations, we find design rules for the geometry and binding energies of our catalyst candidate and derive necessary and sufficient conditions for catalysis which can be directly tested in experiment. Our results open the door to the design of self-regulated artificial systems with bio-inspired functionalities and pave the way towards a better understanding of enzymes.

Thursday, July 21, 2022 at 11am

Heinzel Seminar Room / Office Building West

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