Seminar/Talk

Invisible yet Critical — Hidden Polymorphs, Pre-Nucleation Clusters, and their Role in Molecular Crystallization

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Host: Carl Goodrich

Predicting crystal structures of molecules is a formidable challenge in computational chemistry. Current methods focus on identifying crystal structures with low free energy but are computationally costly and often predict hundreds of structures that are never realized in experiments. In this talk, I will discuss our recent computational efforts [1,2] to uncover the kinetic factors responsible for polymorph selection and amorphization. I will show that the crystals of a large family of coarse-grained molecules can be accurately predicted by incorporating attachment rates of pre-nucleation clusters into classical nucleation theory. I will discuss how this approach can be used to improve conventional energy-based prediction of crystal structures of real molecules, including drug-like organic molecules.[1] Carpenter & Gruenwald, J. Am. Chem. Soc. 2020, 142, 24, 1075510768, https://pubs.acs.org/doi/abs/10.1021/jacs.0c02097[2] Carpenter & Gruenwald, J. Am. Chem. Soc. 2021, 143, 51, 2158021593, https://doi.org/10.1021/jacs.1c09321

Thursday, July 13, 2023 11:00am - 12:00pm
Sunstone Bldg / Ground floor / Big Seminar Room B / 63 seats (I23.EG.102)

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