Unbiased Structure Prediction of Molecular Cages

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Self-assembled cages show promise in a variety of applications (e.g., drug delivery, catalysis, separation, and sensing) due to their structural tunability toward a target problem. Computational cage structure prediction has made significant strides by evaluating possible cage structures from a known library. However, to design and discover novel structures, the community must be able to evaluate and model all candidates without the bias of what has been seen before. Here, we introduce an easy-to-use unbiased structure prediction solution, facilitated through connection with exploration algorithms and our low-cost minimal models in our new software cgx (https://cgexplore.readthedocs.io/en/latest/).

By benchmarking to experiments, we show that our approach predicts existing cage structures starting only from the experimental inputs (building blocks and their stoichiometry). We have used this approach to predict the stoichiometry and structure of heteroleptic cages and host guest systems, and explore pathways and intermediates of self-assembly outcomes. We demonstrate the utility of this method prior to any costly experimental commitment, providing an efficient automated approach that is open source and applicable to multiple model resolutions.