Furukawa Group Seminar

Date

Oct. 6th, 2023
16:00–17:00

Venue

Kyoto University, KUIAS
iCeMS Main Building

2F Seminar Room
(#A207)

Registration

· Required from Google form
(https://forms.gle/cNvqhiCq7b4GKcEQ9)

· On-site only

Contact

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Coarse-grained modelling for molecular materials design

Dr. Emma Wolpert

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Abstract

Coarse-grained models are widely used to reduce the computational cost of simulating materials phase behaviour whilst retaining the main chemical and physical degrees of freedom. But beyond reducing computational cost, coarse-grained models can also be used to develop design rules by highlighting the degrees of freedom which are responsible for materials phase behaviour. Here we show how coarse-grained models can be used for molecular materials design by investigating the supramolecular assembly of porous organic cages. Our results show that by manipulating the parameters of our coarse-grained model, we can reproduce the phase space spanned by porous organic cages found within the literature. By mapping the coarse-grained phase space back onto calculated intermolecular interactions, we can directly relate each cage to its likely crystal packing structure, highlighting the potential for this model to predict the packing of new cages, inform design rules, and motivate targeted cage design. The principle used in this study is not unique to porous organic cages and we showcase examples of how coarse-grained modelling can be used for materials design in other molecular materials.

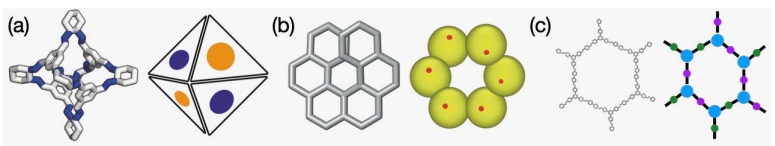

Figure. (Left) atomistic and (right) coarse-grained representation of (a) the porous organic cage CC3 (b) the chiral organic semiconductor [6]helicene, and (c) a multicomponent covalent organic framework.

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