Monte Carlo simulation in de novo design

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The idea of de novo design is to construct new molecular structures for a target application by building up from simple fragments while testing against a cost function. We have used this method for designing templating agents for microporous materials. Here the cost function is simply the interaction energy of the template with its host structure and we find that the candidate molecules produced match well with the known templates used in synthetic chemistry. To compare the candidate templates we have introduced Monte Carlo sampling of configurational space for the molecules in between the building steps. The same techniques have been applied to construction of models for amorphous polymers where the structures generated can be used to understand the hydrogen storage properties of these materials.