Evolving beyond MOFs: evolutionary algorithms for porous organic molecules

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Intrinsically porous organic molecules have shown promise in separations, catalysis, encapsulation, sensing, and as porous liquids. We have been developing an evolutionary algorithm targeted upon the discovery of optimal structures and properties for porous molecular materials. These molecules are typically synthesised from organic precursors through dynamic covalent chemistry (DCC). If we consider cages synthesised from imine condensation reactions alone, there are approximately 800,000 possible aldehyde and amine precursors, combining these in all the different possible topologies results in over 830 million possible porous organic cages. Therefore, either from a computational or synthetic perspective, it is not possible for us to screen all these possible assemblies. Our evolutionary algorithm automates the assembly of hypothetical molecules from a library of precursors. The software belongs to the class of approaches inspired by Darwin's theory of evolution and the premise of "survival of the fittest". Our approach has already suggested promising targets, with preliminary evidence of their synthetic realisation. We are now focusing on predicting optimal organic cage targets for a range of applications such as encapsulation and separation. Further, we are addressing questions such as which topologies or DCC reactions maximise void size or whether specific chemical functionalities promote targeted applications.