Remembering the lab in computational molecular material discovery

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We have been developing computational software towards assisting in the discovery of molecular materials with targeted structures and properties. While initially we have focused upon porous molecular materials, we will also address the ways in which our approach is generalisable to other molecular materials and their applications, including as organic semiconductors or for photocatalysis. Our evolutionary algorithm automates the assembly of
hypothetical molecules from a library of precursors. Our approach has already suggested promising targets that have been synthetically realised. We have also examined the application of both supervised machine learning and explainable graph neural networks for the rapid prediction of porous molecules' properties. Finally, we have trained a model (the Materials Precursor Score, MPScore) to guide our predictions to select materials that have a high chance of being synthesisable in the laboratory. We will also discuss our experimental work to gather data for improved models. Our EPSRC AI hub for Chemistry's (AIchemy) goals and research will also be discussed.