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Theoretical Chemistry Colloquium

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RCMS, 2nd floor, Chemistry Gallery

AuToGraFS: Automatic Topological Generator for Framework Structures

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Abstract: Metal-Organic Frameworks (MOFs) and Covalent-Organic Frameworks (COFs) are recently notable examples of highly porous polymer frameworks with a raft of potential applications in fields as broad as gas separation, sensing, storage and catalysis. Synthesis of these compounds is modular, with connectors and linkers able to be replaced almost at will in the fabrication of isoreticular frameworks - frameworks with the same underlying topology.

The range of components available to form such framework structures is vast, leading to a combinatorial explosion problem in predicting which framework compounds might have a set of desired properties. Computational screening can be used to predict those frameworks that might be usefully synthesised and also to explain the behaviour and properties of already synthesised frameworks. However, both these types of study rely on accurate structural models.

In this work, we present our software; AuToGraFS[1], Automated Topological Generator for Framework Structures and show how it can be used in "computational reticular chemistry". AuToGraFS extends the Python Atomistic Simulation Environment (ASE)[2]

References:

1. Addicoat et al. J. Phys. Chem. Submitted, Addicoat et al. J. Chem. Theory Comput., 10, 880-891 (2014)
2. Bahn, S. R. and Jacobsen, K. W. Comput. Sci. Eng., 4, 56-66, (2002)

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