RCMS Research Center for Materials Science, Nagoya University

Nagoya University

Theoretical Chemistry Colloquium

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RCMS, 2nd floor, Chemistry Gallery

A computational toolkit for mass-screening metal-organic frameworks

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Abstract: *Metal-organic frameworks (MOFs) are a subject of global research attention due to their tunable porous structure, yielding promising applications in the fields of gas storage and separation, catalysis, sensing, etc. The many millions of possible MOFs mean that some form of rapid computational pre-screening is necessary in order to develop MOFs for specific applications.*

We have developed MOF-UFF[1], an extension to Rappe et al.'s Universal Force Field (UFF).[2] MOF-UFF adds several additional atom types that accurately describe the unique metal geometries found in commonly employed SBUs, including those in the IRMOF series, the MIL series and several others.

References:

1. *Akter, I. F., Vankova, N., Addicoat , M. & Heine, T. Manuscript in preparation*
2. *Rappe, A. K., Casewit, C. J., Colwell, K. S., Goddard, W. A. & Skiff, W. M. J. Am. Chem. Soc. 114, 10024–10035 (1992).*

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