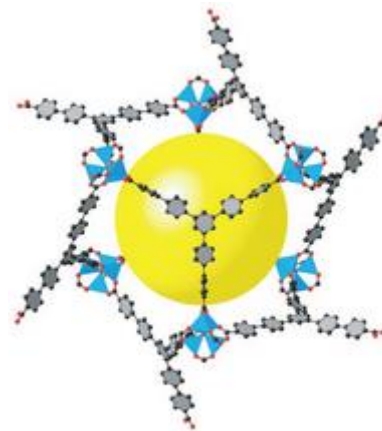


# Introduction to Metal-Organic Frameworks (MOF)

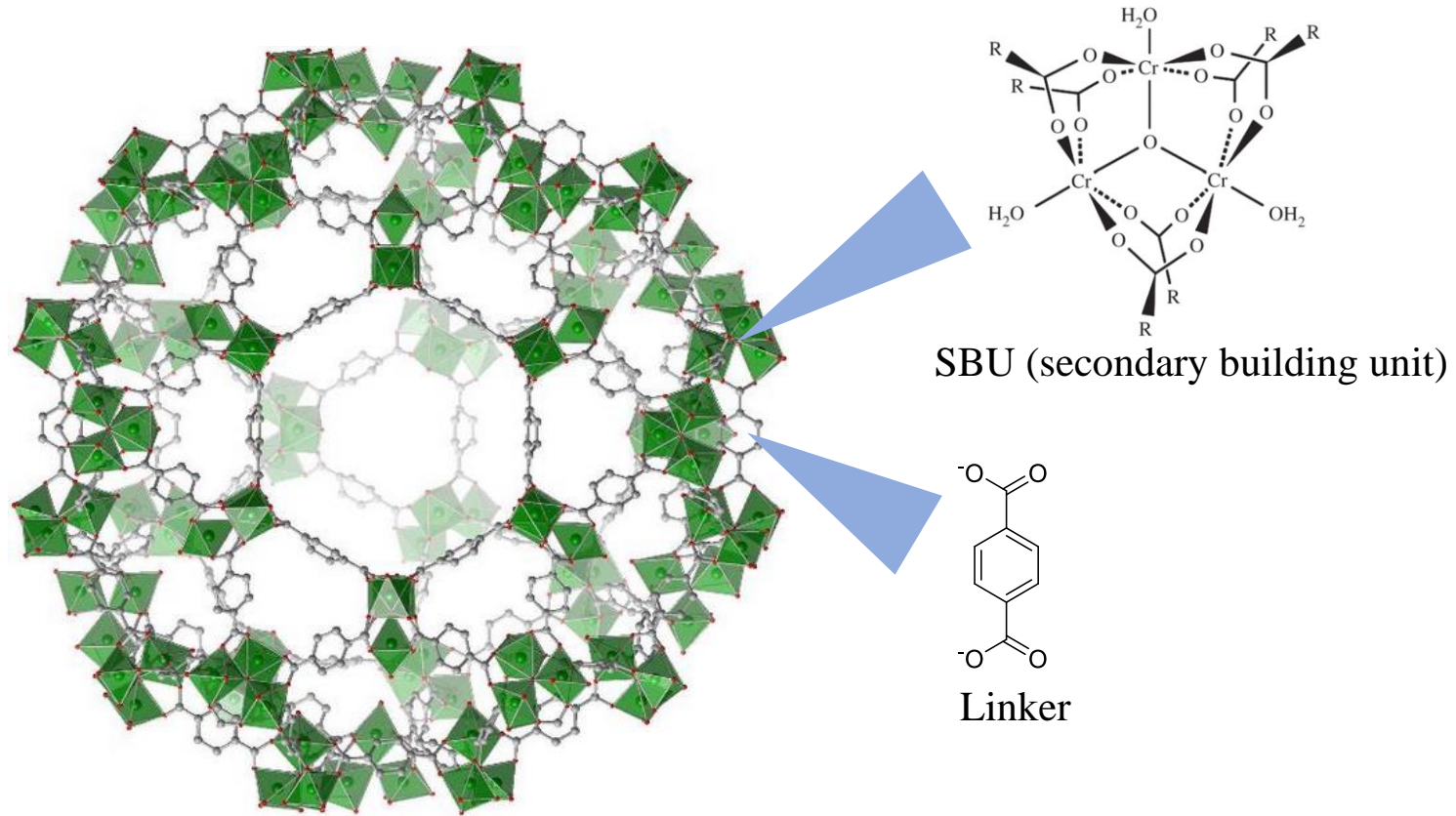


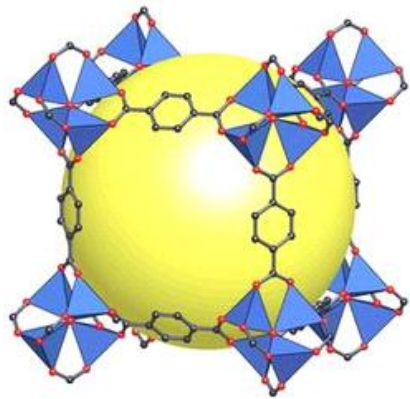
MOF-200

*Science* **2010**, 329, 424

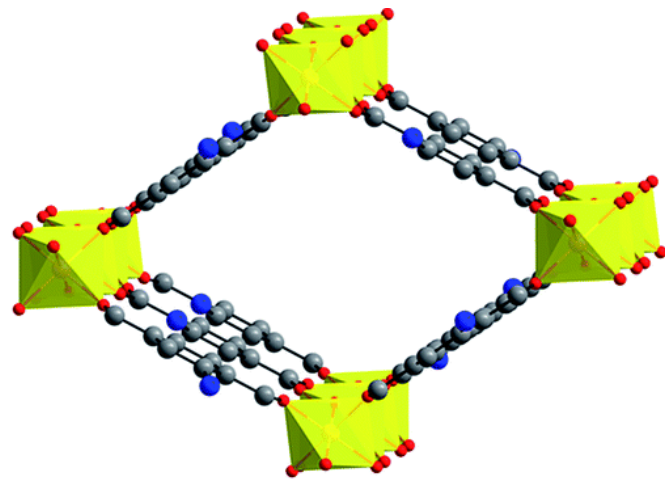
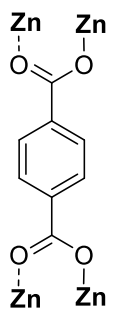
Rihards Kluga  
Rihards.kluga@lu.lv  
27.10.2018

# Metal organic framework

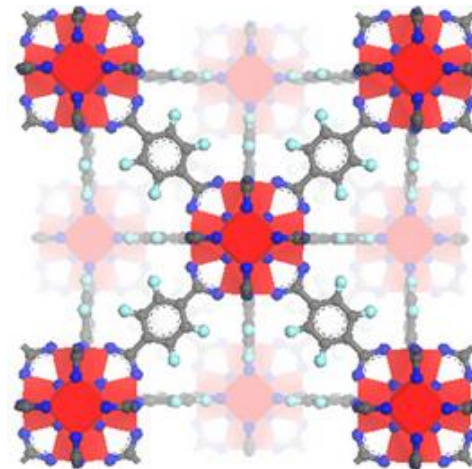
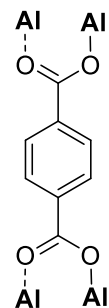




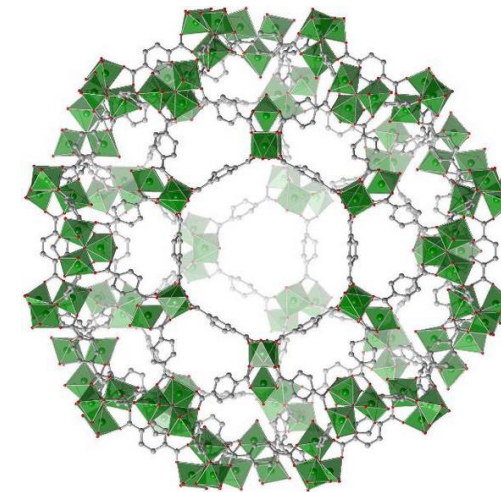
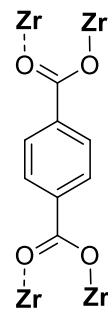
MOF-5



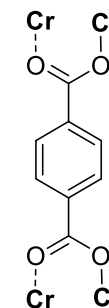
MIL-53(Al)



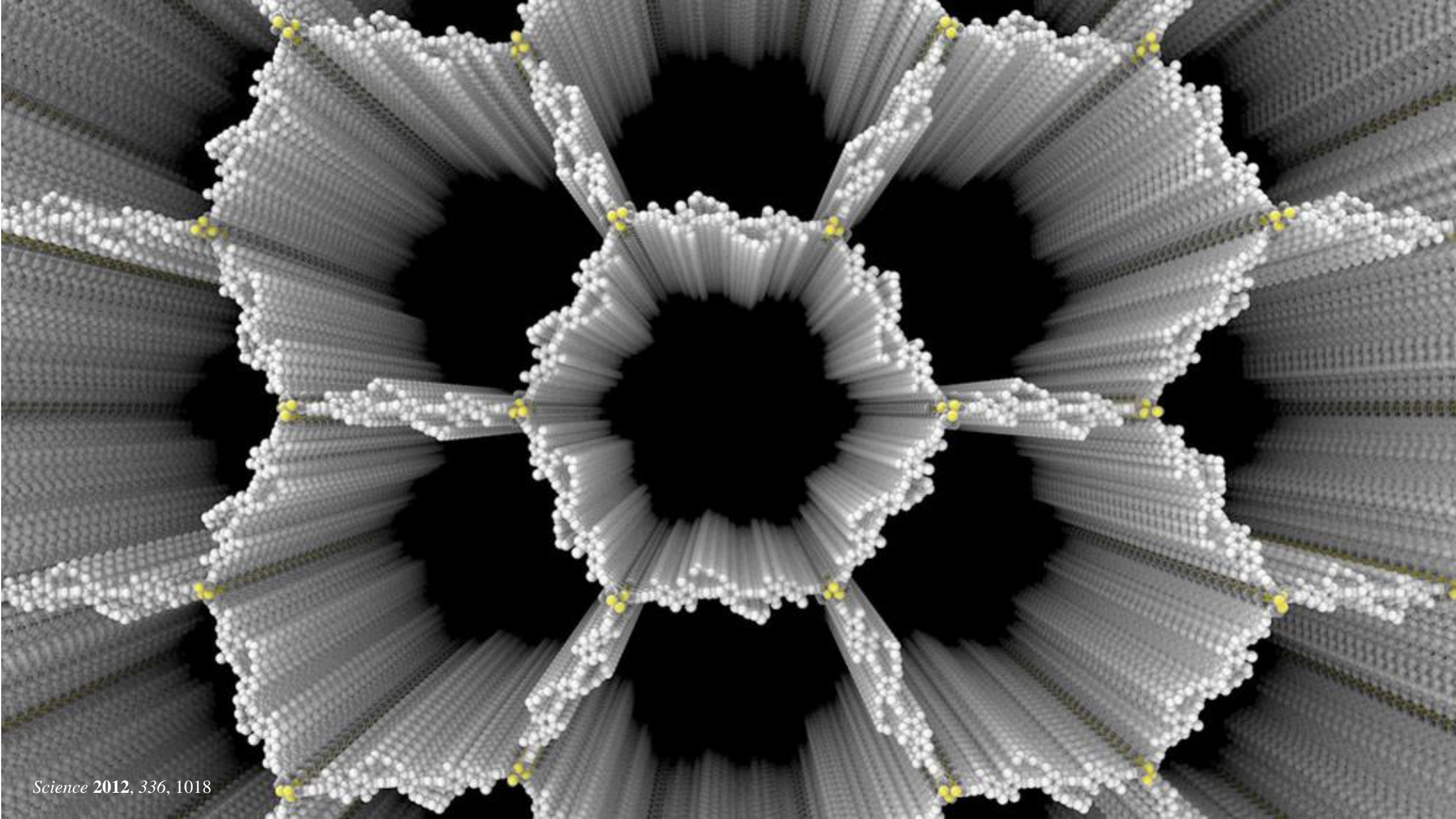
UiO-66



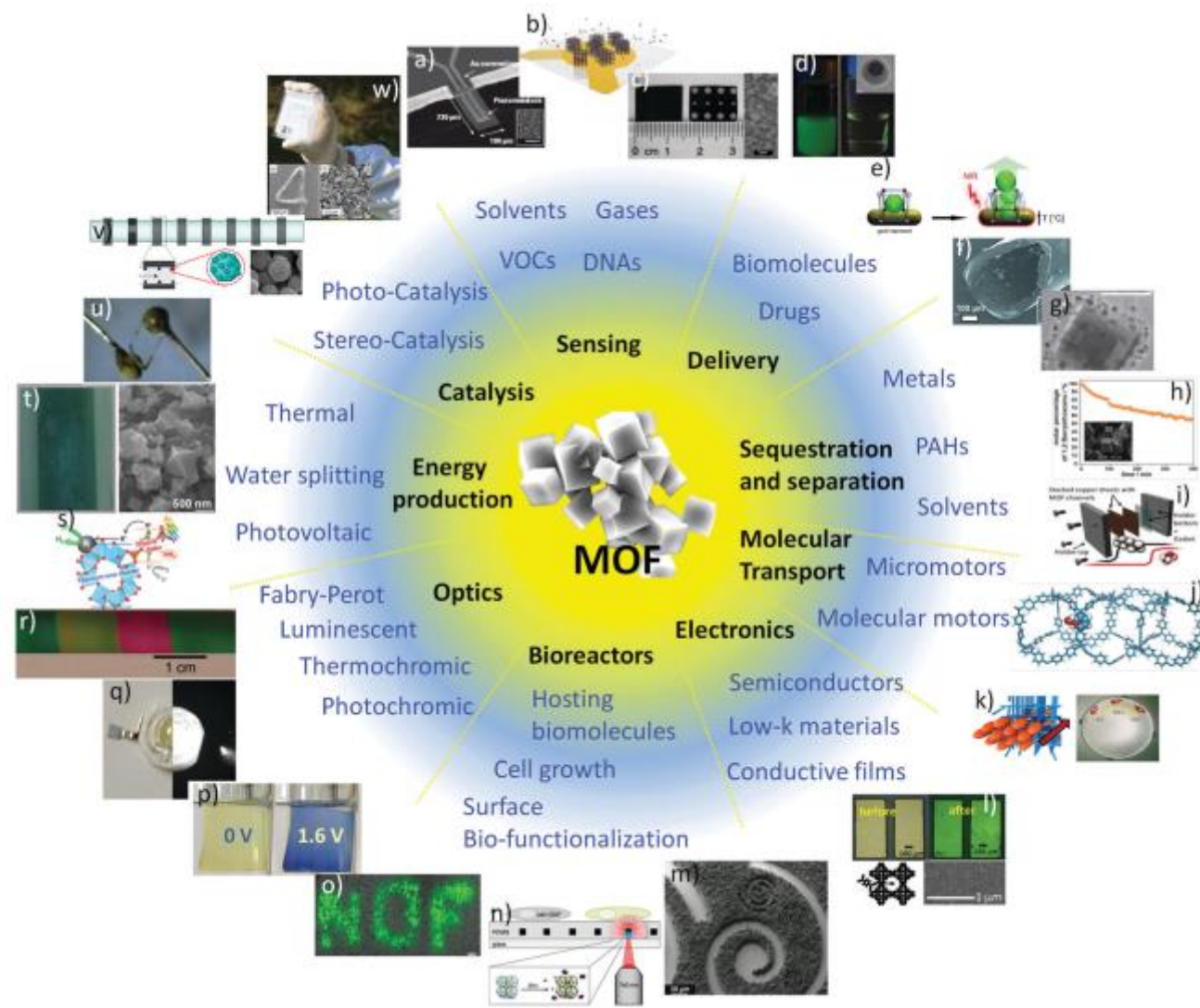
MIL-101(Cr)



*J. Am. Chem. Soc.* **2000**, *122*, 1391; *Science* **2003**, *300*, 1127  
*Chem. Commun.* **2013**, *0*, 2976  
*J. Am. Chem. Soc.* **2008**, *130*, 13850  
*Science* **2005**, *309*, 2040



# Applications



# Force-Field Prediction of Materials Properties in Metal-Organic Frameworks

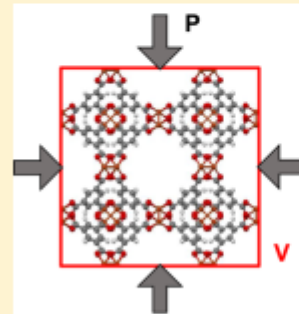
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<sup>†</sup>Laboratory of Molecular Simulation, Institut des Sciences et Ingénierie Chimiques, Ecole Polytechnique Fédérale de Lausanne (EPFL), Rue de l'Industrie 17, CH-1951 Sion, Valais, Switzerland

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**S** Supporting Information

**ABSTRACT:** In this work, MOF bulk properties are evaluated and compared using several force fields on several well-studied MOFs, including IRMOF-1 (MOF-5), IRMOF-10, HKUST-1, and UiO-66. It is found that, surprisingly, UFF and DREIDING provide good values for the bulk modulus and linear thermal expansion coefficients for these materials, excluding those that they are not parametrized for. Force fields developed specifically for MOFs including UFF4MOF, BTW-FF, and the DWES force field are also found to provide accurate values for these materials' properties. While we find that each force field offers a moderately good picture of these properties, noticeable deviations can be observed when looking at properties sensitive to framework vibrational modes. This observation is more pronounced upon the introduction of framework charges.



$$K = -V \frac{dP}{dV} = \text{Bulk Modulus}$$

$$K_{FF} = K_{DFT} \pm 5\%$$

$$FF = \begin{cases} \text{UFF} \\ \text{Dreiding} \\ \text{BTW-FF} \\ \text{UFF4MOF} \\ \text{DWES} \end{cases}$$

# MD simulations of metal-organic frameworks for gas mixture separation

