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"Simulation, design and crystal engineering of metal-organic frameworks"

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Presentation Title: "Force Field Validation for Molecular Simulations of IRMOF-1 and Other Isoreticular Zinc Carboxylate Coordination Polymers"

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We recently developed a non-bonded force field suitable for IRMOF-1 (MOF-5) by combining parameters from a general purpose organic force field (CVFF) with nonbonded parameters for Zn-O interactions.[1] The organic linker is treated as a bonded, flexible species, but inorganic ions (Zn and O) interact only via nonbonded (van der Waal and electrostatic terms). Compared to the rigid framework models used in Monte Carlo simulations of IRMOF-1, our force field includes the effects of framework flexibility suitable for use in both molecular dynamics (MD) and Monte Carlo (MC) simulations. The importance of framework flexibility on gas adsorption and diffusion within the IRMOF-1 pore has been shown using a fully bonded but flexible force field.[2] Because Zn and O ions are not tethered by bond or angle constraints in our force field, . Framework stability in different chemical environments can be studied. For example, we have shown that IRMOF-1 is stable in water up to 2.3 % (w/w) H_2O, but at higher water content the framework collapses. Here we provide further validation of our force field, including compressibility and thermal expansion data, vibrational power spectra, and liquid sorption studies to obtain free volume and self-diffusion coefficients.

Key References

[1] J.A. Greathouse and M.D. Allendorf, *J. Am. Chem. Soc.* **128**, 10678 (2006).
[2] S. Amirjalayer, M. Tafipolsky, and R. Schmid, *Angew. Chemie Int. Ed.* **46**, 463 (2007).