Leveraging Quantum-Chemical In Silico Techniques To Determine Guest Binding Energies for the Crystalline Sponge Method

Timothy Ramadhar[1], Ashley Cardenal[2]

[1]Howard University [2]Howard University

timothy.ramadhar@howard.edu

The crystalline sponge method presents a means to perform single-crystal X-ray diffraction (SC-XRD) analysis on non-crystalline samples [1,2]. The design of new crystalline matrices is necessary to expand the scope and generality of the technique. Computational analysis of crystalline sponge systems provides a way to gain a quantifiable and more detailed understanding of host-guest interactions than through in crystallo analysis alone. Gas-phase geometry optimization and single point energy calculations were performed on existing host-guest metal-organic framework (MOF) complexes based on {[(ZnX2)3(tpt)2]•x(solvent)}n (tpt = tris(4-pyridyl)-1,3,5-triazine, X = I, Br, Cl) to determine guest binding energies [3]. The geometries of the computed gas-phase structures closely matched experimentally-obtained structures. Calculated binding energies were related with guest B-factors to further analyze host-guest interactions. These insights may provide an impetus for further computational studies that will benefit crystal sponge design and selection via virtual screening.

Reference:

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