Supporting Information for:

Understanding Stable Adsorption States in Flexible Soft Porous Coordination Polymers through Free Energy Profiles

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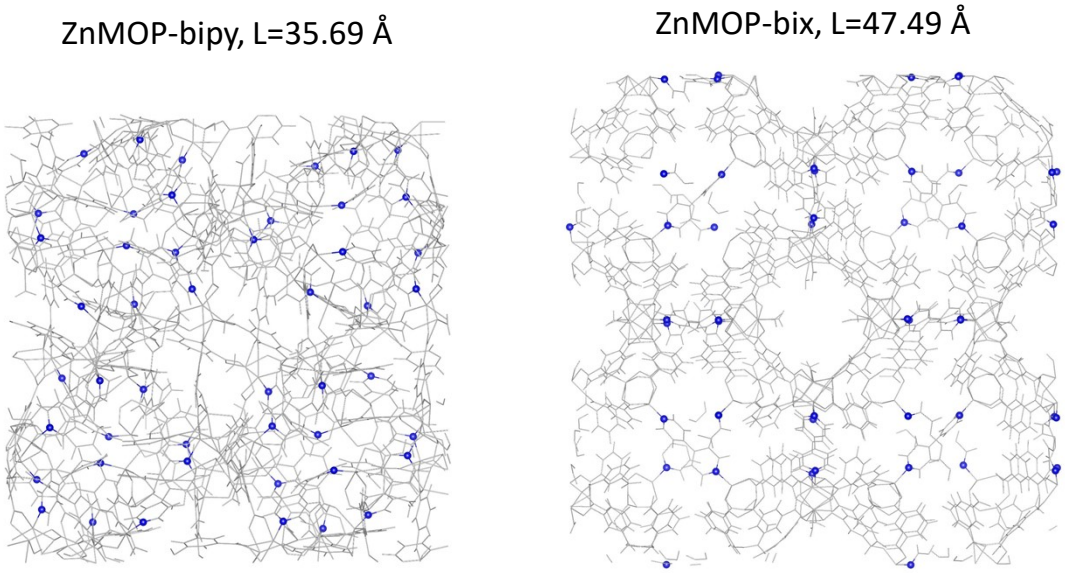

Figure S1: Visualization of crystalline ZnMOP-bipy system at the various free energy minima that appear in **Figure 3**. Highlighted in blue are the nitrogen atoms present in each bipyridine linker.

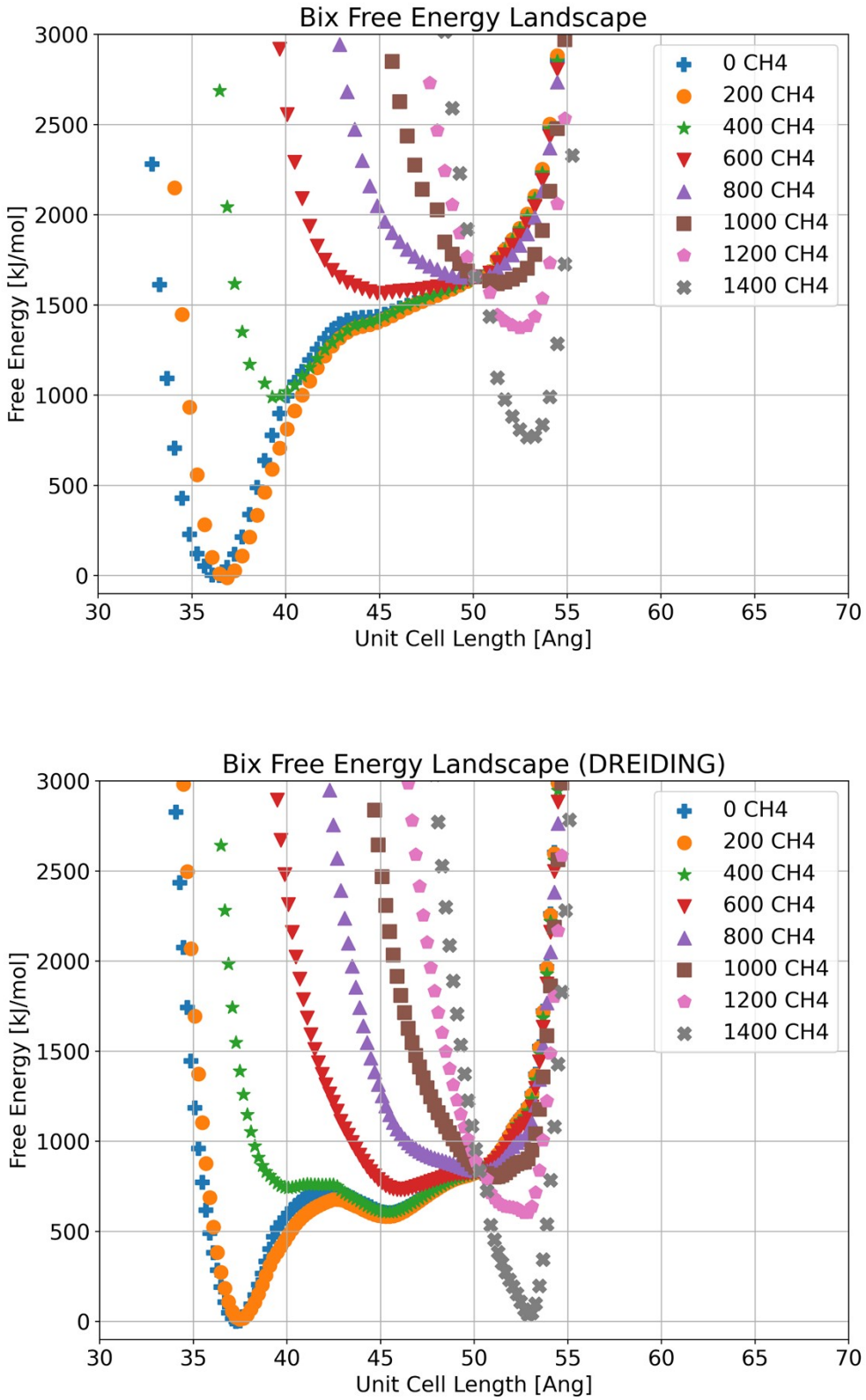

Figure S2: Free energy landscape of the ZnMOP-bix system. Above is reproduced the profile in the main paper, using UFF4MOF, and below is a profile created using the DREIDING force field.

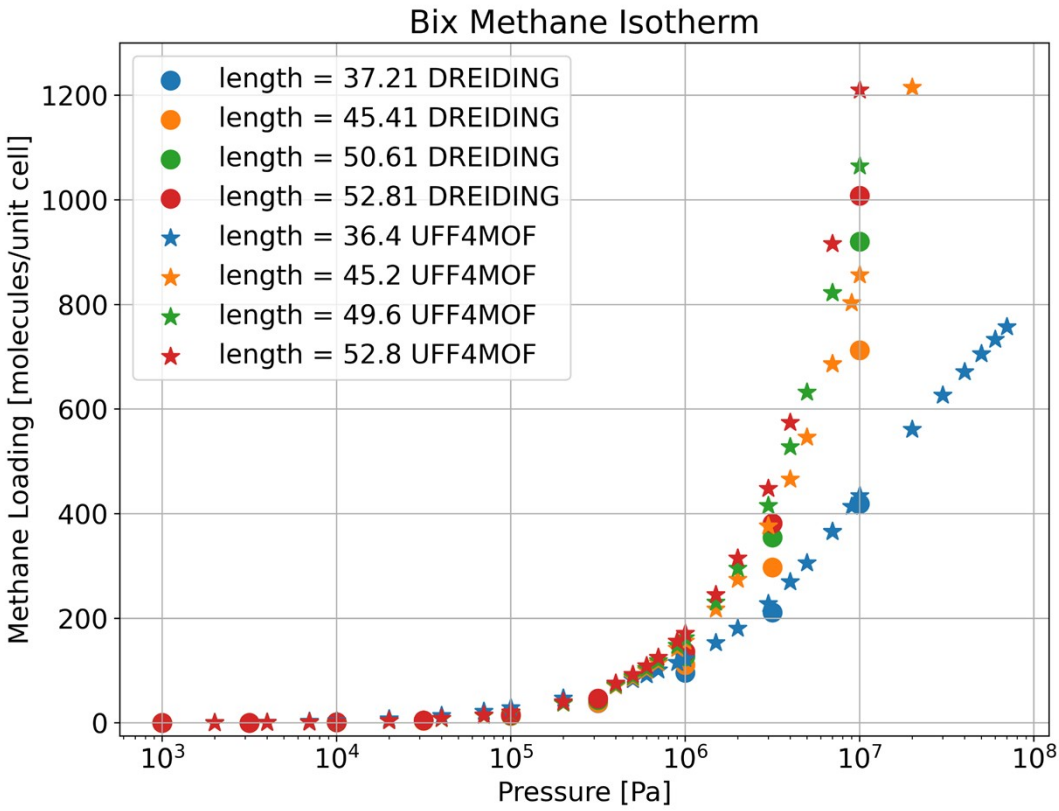

Figure S3: Methane adsorption isotherm of the ZnMOP-bix system at various unit cell lengths (in Angstroms), with a comparison of the isotherm using UFF4MOF and DREIDING.

Looking at **Figure S2** we see agreement in the positions of the closed pore and open pore states using either the UFF4MOF or DREIDING [61] force fields. We also see the shift from closed pore to transition to open pore phases at the same loadings, though we do see more clearly a free energy well corresponding to the transition at a unit cell side length of approximately 45 Å.

In **Figure S3** we compare adsorption isotherms of the same two systems and see agreement between the two force fields.

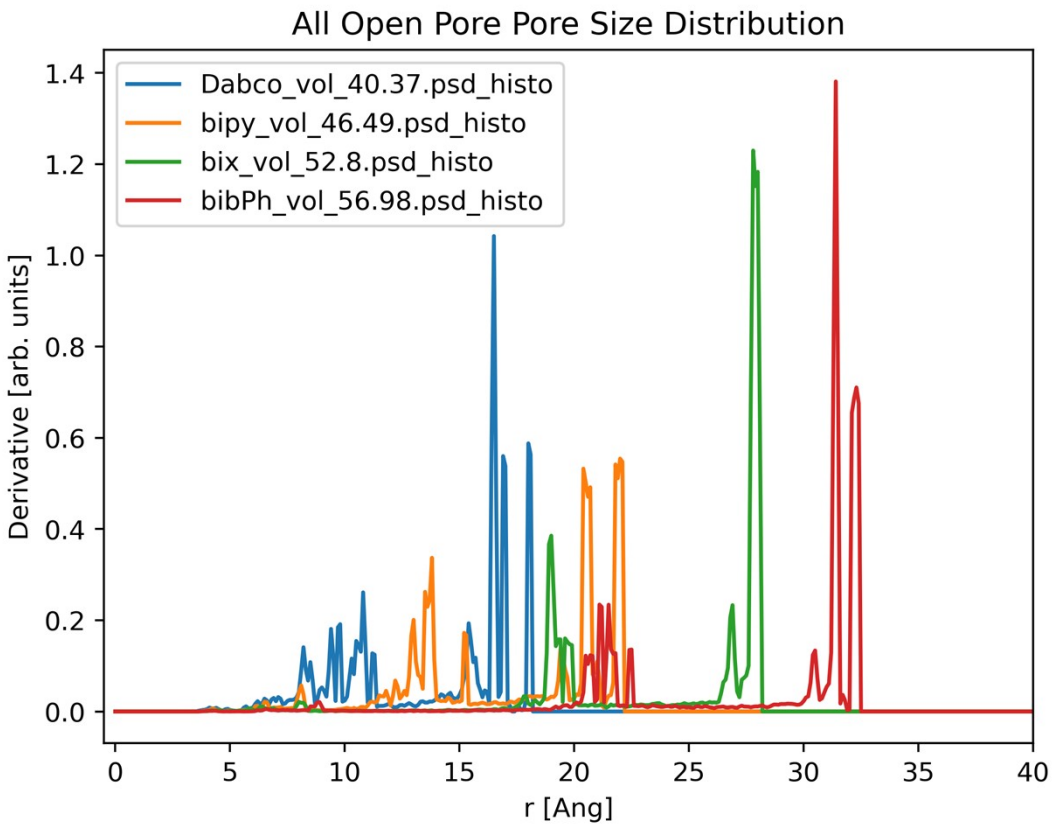

Figure S4: Pore size distributions for each system (Dabco, bipyridine, bix, and bibPh) in their most open configuration.