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5-fold increase of hydrogen uptake in MOF74 through linker decorations[1] T. THONHAUSER, S. ZULUAGA, D. HARRISON, E. WELCHMAN, C. ARTER, Wake Forest University — We present *ab initio* results for linker decorations in Mg-MOF74—i.e. attaching various metals $\mathcal{M}$ = Li, Na, K, Sc, Cr, Mn, Fe, Ni, Cu, Zn, Rb, Pd, Ag, and Pt near the ring of the linker—creating new strong adsorption sites and thus maximizing small molecule uptake.[2] We find that in most cases these decorations influence the overall form and structure of Mg-MOF74 only marginally. After the initial screening we chose metals that bind favorably to the linker and further investigate adsorption of H_2, CO_2, and H_2O for $\mathcal{M}$ = Li, Na, K, and Sc. For the case of H_2 we show that up to 24 additional guest molecules can be adsorbed in the MOF unit cell, with binding energies comparable to the original open-metal sites at the six corners of the channel. This leads to a 5-fold increase of the molecule uptake in Mg-MOF74, with tremendous impact on many applications in general and hydrogen storage in particular—where the gravimetric hydrogen density increases from 1.63 mass% to 7.28 mass% and the volumetric density from 15.10 g H_2 L^{-1} to 75.50 g H_2 L^{-1}.

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[2]C. Arter, S. Zuluaga, D. Harrison, E. Welchman, and T. Thonhauser, Phys. Rev. B **94**, 144105 (2016).

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