Electronic Supplementary Material for PCCP


# Supplementary Information

## Enhanced Dihydrogen Adsorption in Symmetry-Lowered Metal-Porphyrin-Containing Frameworks

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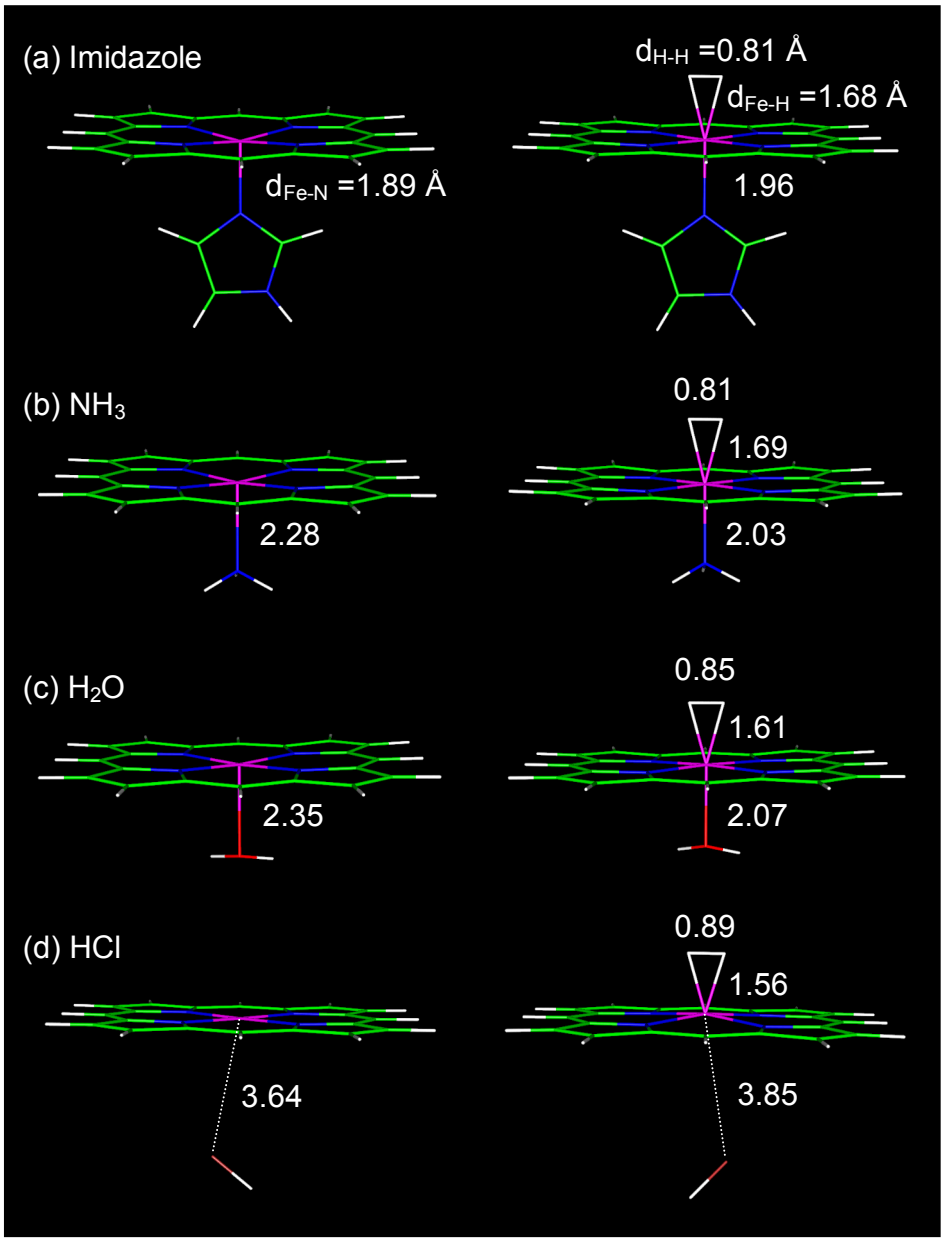


**Fig. S1.** Atomic geometries of high-spin Fe-porphyrin-ligands (left) and low-spin $H_2$-Fe-porphyrin-ligands (right): Green (C), white (H), blue (N), magenta (Fe), red (O), and brown (Cl).

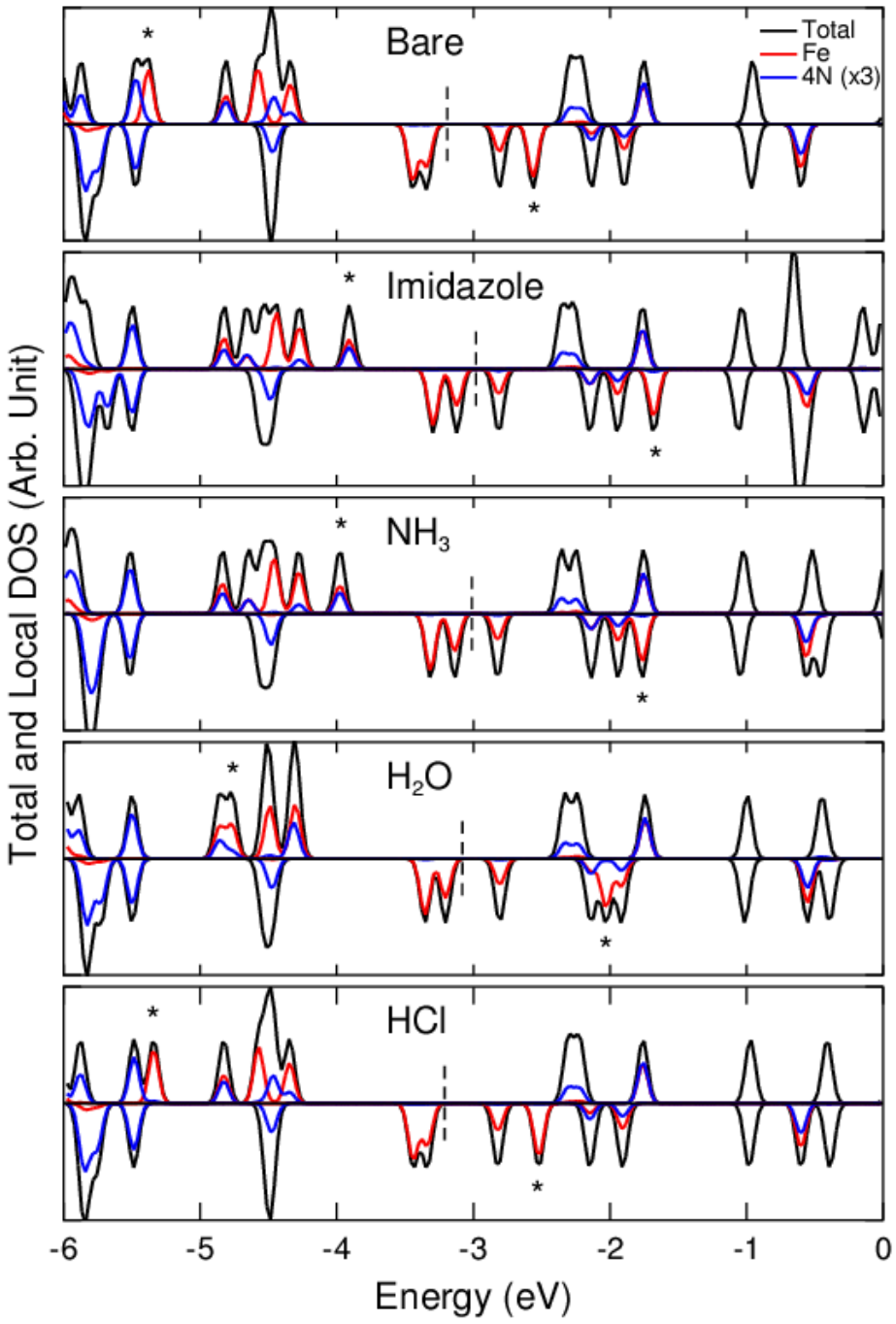


**Fig. S2.** Total and local spin density of states (DOS) of high-spin (S=1) Fe-porphyrins with different symmetry-breaking ligands near the highest occupied molecular orbitals (marked by dashed lines). Local DOS is projected onto Fe (in red) and four N's (in blue and multiplied by 3) of the porphyrin. The energy is Kohn-Sham as calculated with the core-level alignment. The $d_{z2}$ orbital is marked with (*).