

Insights into the Enhanced Activity of a Metal–Organic Framework-Encapsulated Enzyme

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Structural changes of cytochrome c (Cyt c) upon encapsulation within a hierarchical metal–organic framework (NU-1000) lead to enhanced catalytic performance.

The encapsulation of enzymes within porous materials is promising to protect the enzymes from denaturation under non-biological environments and to facilitate their enzymatic activity. Here, the structural changes of cytochrome c (Cyt c) upon encapsulation within a hierarchical metal–organic framework (NU-1000) are uncovered using electron paramagnetic resonance, solid state ultraviolet-visible spectroscopies, and atomistic molecular dynamics simulations. The enhanced catalytic performance of Cyt c encapsulated within NU-1000 is attributed to the configurational changes around the heme ferric active center, and supported by the physical and *in silico* observations

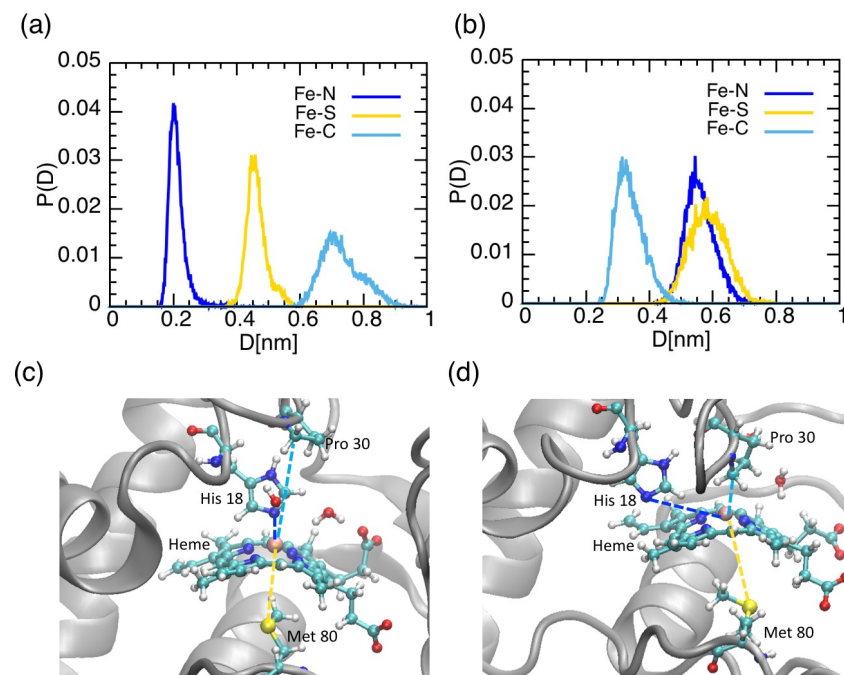


Figure 1: Probability distributions of the distance D of selected nearby atoms (N, S, and C) relative to Fe, (a) in bulk and (b) inside MOF NU-1000. Configurations of Cyt C in water (c) and inside MOF NU-1000 (d).