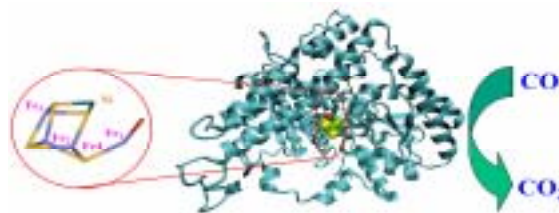

Computational Characterization of Reactive Intermediates of Carbon Monoxide Dehydrogenase

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The catalytic oxidation of CO to CO₂ by carbon monoxide dehydrogenases has been explored theoretically, and a large C-cluster model including the metal core [Ni-4Fe-4S] and surrounding residues and crystal water molecules was used in density functional calculations. The key species involved in the oxidation of CO at C-cluster, C_{red1}, C_{red2} and C_{int}, have been elucidated. On the basis of computational results, the plausible enzymatic mechanism for the CO oxidation was proposed. Predicted geometries of key species show good agreement with the reported crystal structures.
