Numerical Computation of Enzyme Function

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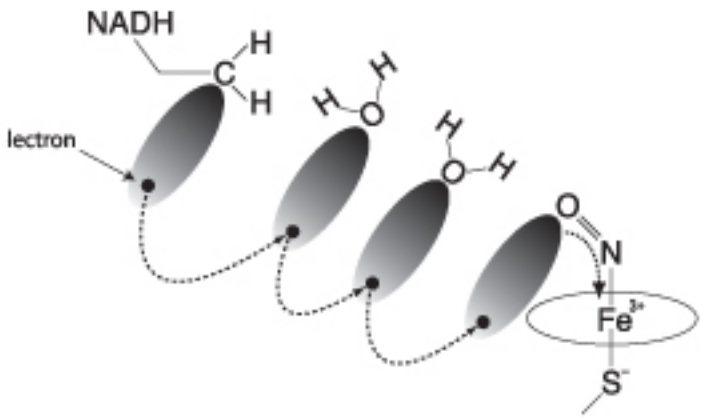
Nitric Oxide reductase (NOR) isolated from the denitrifying fungus *Fusarium oxysporum* is a cytochrome P450-type heme enzyme [1-3]. NOR catalyzes a nitric oxide (NO) reduction reaction in which two NO molecules are converted into a nitrous oxide molecule using two electrons directly transferred from NADH [4].

The reaction path for NO reduction in NOR was obtained using the semiempirical method SAM1 [5].

We analyzed the two electron transfer system that supported the function of NOR using the docking simulation and the quantum chemical calculation. Then, we propose the system that the two electrons transmit as a charged soliton (Figure 1).



Schematic representation of the two electron transfer system, the charged soliton as illustrated by the dashed line