Electron transfer in bacterial photosynthesis: New insights from atomistic theory and simulation

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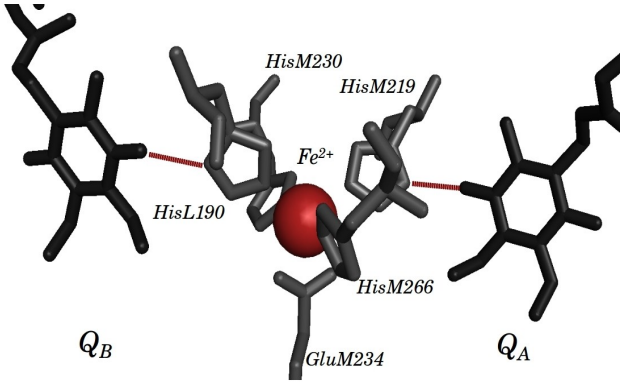
Although the bacterial photoreaction center was the first membrane protein characterized structurally [1], many charge transfer steps in this paradigmatic enzyme still are under a cloud. Here, we use atomistic molecular dynamics simulations and large-scale electronic structure computations to address charge transfer between i) the Q_A and Q_B quinones, ii) four heme centers in the cytochrome subunit and iii) the cytochrome subunit and the bacteriochlorophyll special-pair.



The results show that an extraordinary, hydrogen-bound non-heme iron complex is essential for efficient interquinone charge transfer allowing a bridge-mediated superexchange mechanism [2]. Furthermore, thermodynamic integration calculations enabled the computation of free enthalpy values for the interheme charge transfer in the cytochrome subunit. Additionally, in the final rereduction step of the photooxidized special-pair by the last of the four heme moieties of the cytochrome subunit, several charge transfer pathways involving different amico acids at the protein-cytochrome interface could be identified and it was shown, that the kinetics of these pathways is not affected by photoinduced changes in the protein structure.

[1] J. Deisenhofer, O. Epp, K. Miki R. Huber, H. Michel., *Nature*, **1985**, *318*, 618-624.
[2] F. Burggraf, T. Koslowski., *Biochim. Biophys. Acta*, **2011**, *1807*, 53-58.