Thermodynamic Integration Network Study of Electron Transfer: from Proteins to Aggregates [1]

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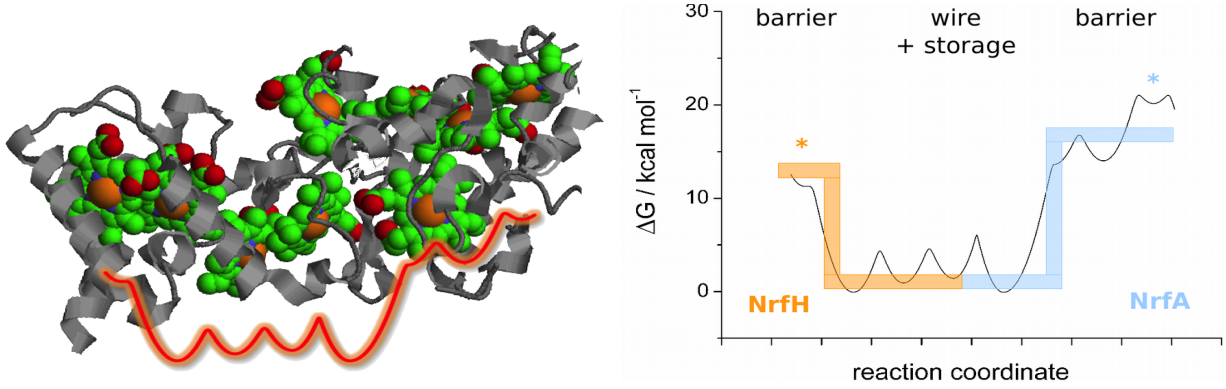

We describe electron transfer through the NrfHA nitrite reductase heterodimer [2] using a thermodynamic integration scheme based upon molecular dynamics simulations. From the simulation data, we estimate two of the characteristic energies of electron transfer, the thermodynamic driving forces, ΔG, and the reorganization energies, λ. Using a thermodynamic network analysis, the statistical accuracy of the ΔG values can be enhanced significantly. Although the reaction free energies and activation barriers are hardly affected by protein aggregation, the complete reaction mechanism only emerges from the simulations of the dimer rather than focussing on the individual protein chains: it involves an isoenergetic transprotein element of electron storage and conductivity [1].

[1] S. Na, A. Bauß, M. Langenmaier, T. Koslowski, *Phys. Chem. Chem. Phys.*, **2017**, *19*, 18938–18947.
[2] M. Rodrigues, K. Scott, M. Sansom, I. Pereira, M. Archer, *J. Mol. Biol.*, **2008**, 381, 341–350.