

P017 Theory of charge transfer in Complex I
– an atomistic perspective

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In this contribution, we describe the electronic structure of the redox chain in complex I with a chemically specific, atomistic model that has been carefully parameterized using quantum chemical ab initio calculations. Our approach accounts for the physics of the chemical bond, polarization effects within the protein medium and spin polarization and local magnetism on Fe. The emerging potential energy surfaces can be analyzed using Marcus' theory of charge transfer, finally leading to charge transfer rates that can be compared to experimental results. We are able to distinguish through space, through bond and intermediate hopping contributions to the charge transfer process. The corresponding rates do not only depend on the intercluster distances, but on their mutual orientation and spin polarization. In addition, we have identified a kinetic bottleneck between the clusters n5 and n6a.