Abstract Submitted
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Computational studies of a redox-driven proton pump: Cytochrome c oxidase and biological energy transduction[1] ALEXEI A. STUCHEBRUKHOV, UC Davis — Cytochrome c oxidase (CcO) is a redox-driven proton pump, an energy converting molecular machine, which reduces atmospheric oxygen to water and couples the oxygen reduction reaction to the creation of a membrane proton gradient. The proton gradient subsequently drives the synthesis of ATP. The structure of the enzyme has been solved; however, the molecular mechanism of proton pumping is still poorly understood. The correlated electron and proton transport plays a crucial role in the function of the enzyme. Our computer simulations – combined ab initio and classical, MD and MC- indicate a possible mechanism of CcO. We find that one of the His ligands of the catalytic site, and certain chains of water molecules inside of the enzyme play a crucial role. In this presentation, computational and experimental studies directed toward understanding the mechanism of cytochrome c oxidase will be discussed. D.M. Popovic and A.A. Stuchebrukhov, Proton pumping mechanism and catalytic cycle of cytochrome c oxidase: Coulomb pump model with kinetic gating, FEBS Lett. 2004.

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