

Reaction Pathways Driving Proton Pumping in Bacterial Class ba3 Cytochrome c Oxidase: A View from Quantum Chemistry and Molecular Dynamics

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Abstract: The terminal electron acceptor of the electron transport chain both in mitochondria and in aerobic bacteria is Cytochrome c Oxidase (CcO). Here electrons and protons react with molecular oxygen at a dinuclear metal (FeCu) center through a catalytic cycle, producing charge separation and proton pumping across the inner membrane. How the energy changes over this reaction cycle are effectively utilized for charge separation and proton pumping still contains many unsolved problems. Using quantum chemistry (DFT) and Molecular Dynamics, we have explored potential reaction pathways in a bacterial CcO. In addition to exploring structures and energy pathways, comparing our DFT predictions with spectroscopies and kinetics helps us find the right paths and reaction mechanisms.