Analysis of the Radiation-Damage-Free X-ray Structure of Photosystem II in Light of EXAFS and QM/MM Data

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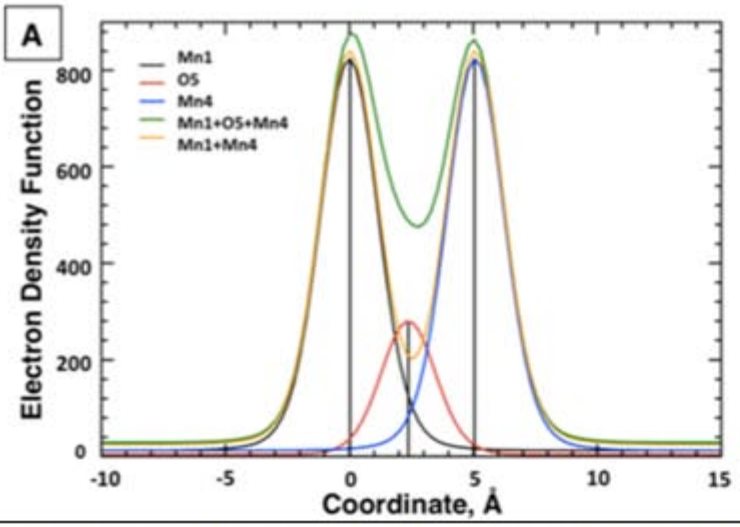

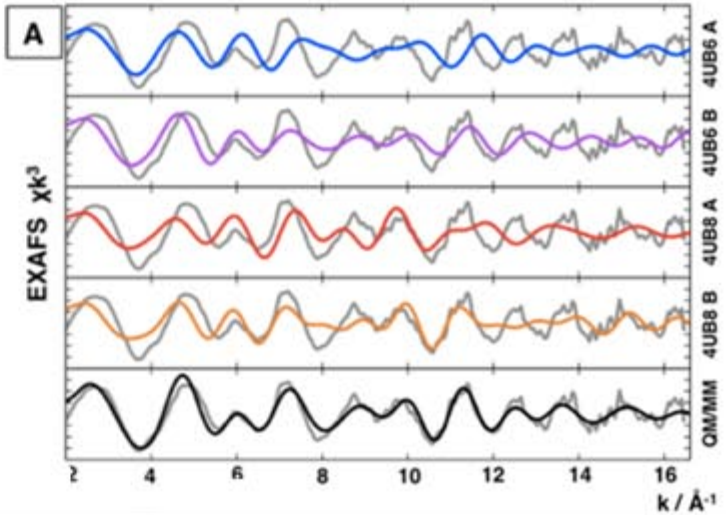

Simulated electron density profile of the Mn1–O5– Mn4 coordinate and EXAFS spectra simulated from 4UB6 monomer A (blue), 4UB6 monomer B (purple), 4UB8 monomer A (red), and 4UB8 monomer B (orange) compared to the experimental S1 spectrum (gray) and DFT-QM/MM (black). O atoms close to Mn centers are difficult to resolve even at 1.95 Å, so their assigned positions are dependent on the model used to fit the e density.