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The Unpaired Electron Spin Density Distribution in Reduced [2Fe-2S] Clusters by $^{13}C_b$-Cysteine Labeling

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Iron-sulfur clusters are some of the most versatile classes of electron transport mediators in biology. The roles of these metal centers are predominantly determined by the coordinating ligands (typically cysteine and histidine) that modify the electronic structure of the cluster. Here we determine the spin density distribution onto the cysteine ligands for the three major classes of the reduced [2Fe-2S](His)$_n$(Cys)$_{4-n}$ (n=0,1,2) cluster by site-specific ^{13}C isotope labeling of the cysteine b-carbons. The spin distribution is asymmetric and delocalizes further along the reducible Fe^{2+} ligands than the Fe^{3+} ligands. The preferential spin transfer onto the chemically reactive Fe^{2+} ligands supports that the orientation of the cluster in proteins is not arbitrarily decided, but rather is optimized for better electronic coupling with redox partners. Finally, the resolution of all cysteine b-carbon ^{13}C hyperfine couplings provides a measure of the relative covalencies of the metal-thiolate bonds not available from other techniques.

Biography:

Alexander Tomoaki Taguchi career as a magnetic resonance spectroscopist began at the University of Illinois at Urbana-Champaign(USA) Biophysics graduate program. He studied photosynthetic reaction centers using pulsed Electron Paramagnetic Resonance to obtain high-resolution insight into the structure-function relationships of the electron transport processes. He then transitioned into the field of iron-sulfur clusters as a postdoctoral fellow at the Nippon Medical School in Tokyo, Japan. Currently he is working as an NIH postdoctoral fellow on solid-state Nuclear Magnetic Resonance fast magic angle spinning on membrane proteins at the Massachusetts Institute of Technology.