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Ab initio studies of $[Fe_4S_4]^{2+/3+}$ clusters in metalloprotein MutY[1]
JONG-CHIN LIN, DANIEL COX, RAJIV SINGH, U.C. Davis — Iron sulfur clusters are present in the DNA repair protein MutY in a region highly homologous in species as diverse as E. Coli and Homo Sapiens, yet their function remains unknown. In MutY, this mixed valence cluster exists in two oxidation states, $[Fe_4S_4]^{2+/3+}$, with the stability depending upon the presence of DNA. We have studied the electronic structure and stability of these clusters using density functional theory, in particular the local orbital based SIESTA program. Our calculation shows that the energy difference between 2+ and 3+ forms is within the range of 0.1eV, which suggests that the redox process is reversible. We use this to propose a possible redox mechanism for modulating the rate for scanning for oxidized G-A mismatches in DNA by MutY [2]. We note that this redox modulation mechanism for site recognition scanning may have broader generality.

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[2]M. Slutsky and L.A. Mirny, preprint q-bio.BM/0402005 at http://arxiv.org.

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