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Structural and electronic properties of copper-containing nitrite reductase (CuNiR): elucidating the mechanism of nitrite reduction at the T_2Cu center YAN LI, MIROSLAV HODAK, JERRY BERNHOLC, North Carolina State University — Copper-containing nitrite reductases (CuNiRs) play an important role in catalyzing the reduction of NO_2^- to NO during the bacterial denitrification process. Experimental studies have provided the structures of various states of CuNiR in the catalytic reaction, but many important aspects of the initial and intermediate attachments as well as the mechanism of the enzyme function remain unclear. We present a density-functional-theory-based study of the structural and electronic properties of different coordination forms at the T_2Cu center. The nudged elastic band (NEB) method is used to examine the activation energy barriers and to determine the minimum energy pathways (MEP) of the reaction processes. Our results reveal the role of the Asp^{98} residue in the enzymatic function of CuNiR and also address the transformation from the initial O-coordinated binding of NO_2^- to the N-coordinated attachment of the NO during the enzymatic reaction.

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