Volume 71 (2015)

Supporting information for article:

Structural insights into the efficient CO2-reducing activity of an NAD-dependent formate dehydrogenase from *Thiobacillus* sp. KNK65MA

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Figure S1  QM region setup for the active site of TsFDH. The corresponding residues of CbFDH are given in parentheses.

Figure S2  Optimized geometries (stereo) of the active site of CbFDH for the CO$_2$ → formate conversion: (a) reactant, (b) transition, and (c) product states. Colored stick models represent the structures optimized with SCC-DFTB and geometries with green color correspond to those optimized with B3LYP/6-31+G(2d,2p). Some important bond lengths and angles are also shown for structures optimized by SCC-DFTB and B3LYP/6-31+G(2d,2p) (in parentheses).
Figure S3  Optimized geometries (stereo) of the active site of TsFDH for the CO$_2$ → formate conversion: (a) reactant, (b) transition, and (c) product states. Colored stick models represent the structures optimized with SCC-DFTB and geometries with green color correspond to those optimized with B3LYP/6-31+G(2d,2p). Some important bond lengths and angles are also shown for structures optimized by SCC-DFTB and B3LYP/6-31+G(2d,2p) (in parentheses). It is noted that Asn119 in these snapshots are hidden by NAD.
Figure S4  Multiple sequence alignment of FDHs. TsFDH (UniProtKB/Swiss-Prot accession number Q76EB7) was aligned with PsFDH (UniProtKB/Swiss-Prot accession number P33160), MsFDH (UniProtKB/Swiss-Prot accession number O08375), AtFDH (UniProtKB/Swiss-Prot accession number Q9S7E4), and CbFDH (UniProtKB/Swiss-Prot accession number O13437). Residues that interact with NAD$^+$ are marked with black dots. Secondary structure elements of TsFDH assigned by PyMOL are indicated above the sequences. Residues that are strictly conserved and partially conserved among these species are shown in green and yellow, respectively. The figure was drawn with ClustalX (Larkin et al., 2007) and GeneDoc (Nicholas et al., 1997).