

Description of Additional Supplementary Files

File Name: Supplementary Data 1

Description: Cartesian coordinates of all optimized structures.

File Name: Supplementary Movie 1

Description: One representative MD trajectory for the uncatalyzed reaction in solution.

File Name: Supplementary Movie 2

Description: One representative MD trajectory for the Fe-catalyzed reaction in the quartet state and six-coordinate form in solution.

File Name: Supplementary Movie 3

Description: One representative MD trajectory for the Fe-catalyzed reaction in the sextet state and five-coordinate form in solution.

File Name: Supplementary Movie 4

Description: One representative MD trajectory for the Fe-catalyzed reaction in the sextet state and five-coordinate form in solution in the presence of the oriented external electric field (OEEF).