Photoinduced water splitting with oxotitanium porphyrin: a computational study

Andrzej L. Sobolewski and Wolfgang Domecke

Electronic Supplementary Information
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Fig. S1. The Kohn-Sham frontier orbitals of the TiPOH' radical at the equilibrium geometry of the $^2A_1$ state ($R_{OH} \approx 1.0$ Å, left column) and at the dissociation limit ($R_{OH} = 2.7$ Å, right column). Only one component of the degenerate ($e$) orbitals is shown.
Cartesian coordinates (in Ångstrom) of the $S_0(C_{4v})$ equilibrium geometry of TiOP optimized with the DFT/B3LYP/cc-pVDZ(TZVP at Ti) method.

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Cartesian coordinates (in Ångstrom) of the $S_0(C_I)$ equilibrium geometry of the TiOP-H$_2$O complex optimized with the DFT/B3LYP/cc-pVDZ(TZVP at Ti) method.

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Cartesian coordinates (in Ångstrom) of the $^1$LMCT($A'$) inner minimum geometry of the TiOP-H$_2$O complex optimized with the DFT/B3LYP/cc-pVDZ(TZVP at Ti) method.

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Cartesian coordinates (in Ångstrom) of the $^2B_1$ minimum geometry of the TiPOH$^\bullet$ radical optimized with the DFT/B3LYP/cc-pVDZ(TZVP at Ti) method.

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