
Supporting Information

Effect of Water Molecule on Photoassisted Nitrous Oxide Decomposition over Oxotitanium Porphyrin: A Theoretical Study

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	Page
I. Figure S1. Absorption spectrum of TiO-Por and N ₂ O calculated by TD-M06L method.	S2
II. Figure S2. Relevant MOs (a) HOMO-1, (b) HOMO, (c) LUMO, and (d) LUMO+1, of TiO-Por upon excitations.	S2
III. Figure S3. Spin density plot of triplet state TiO-Por.	S3

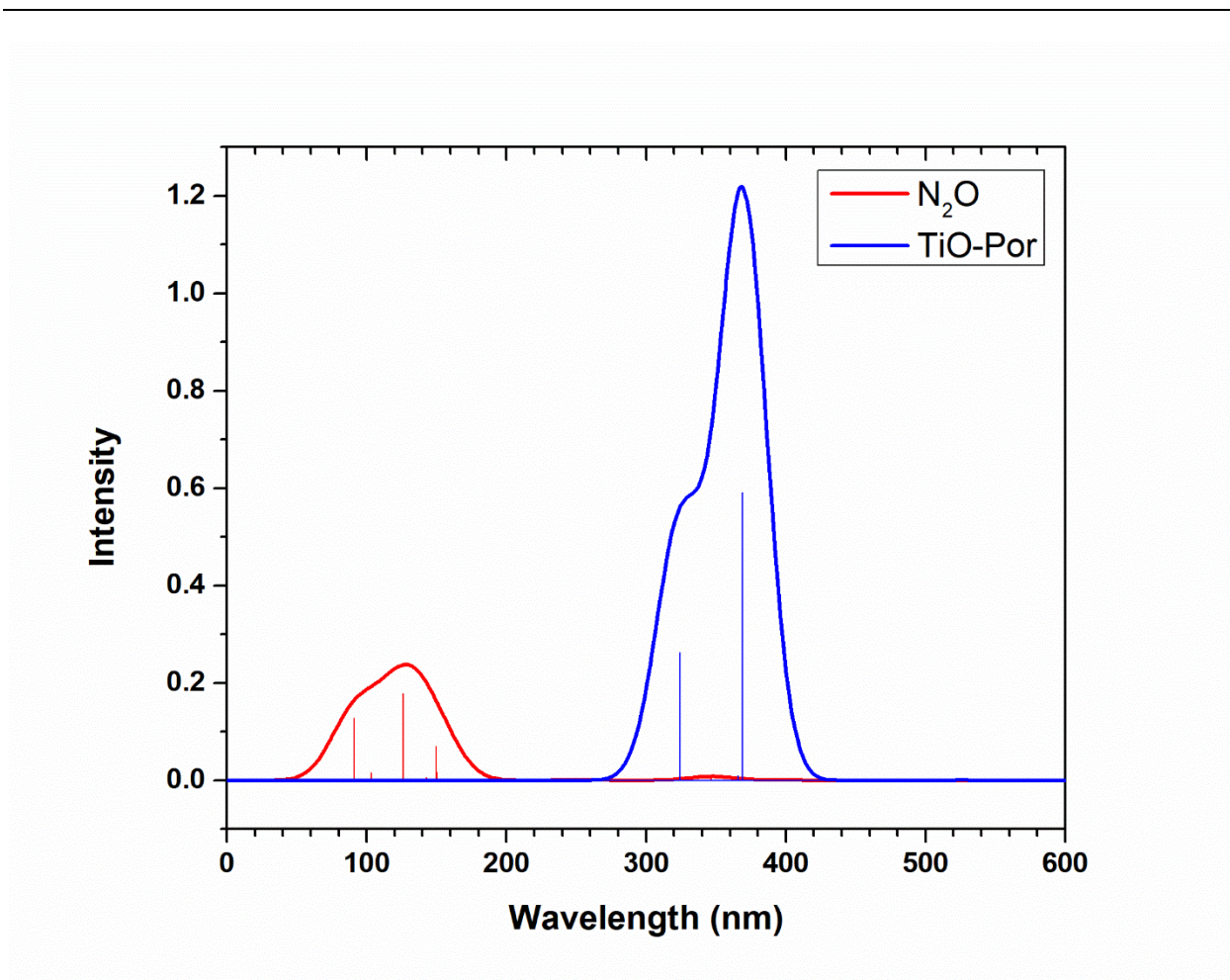


Figure S1. Absorption spectrum of TiO-Por and N₂O calculated by TD-M06L method.

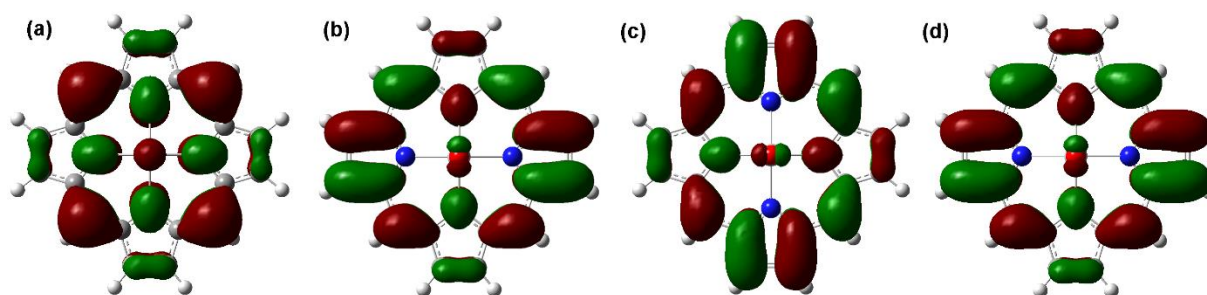


Figure S2. Relevant MOs (a) HOMO-1, (b) HOMO, (c) LUMO, and (d) LUMO+1, of TiO-Por upon excitations.

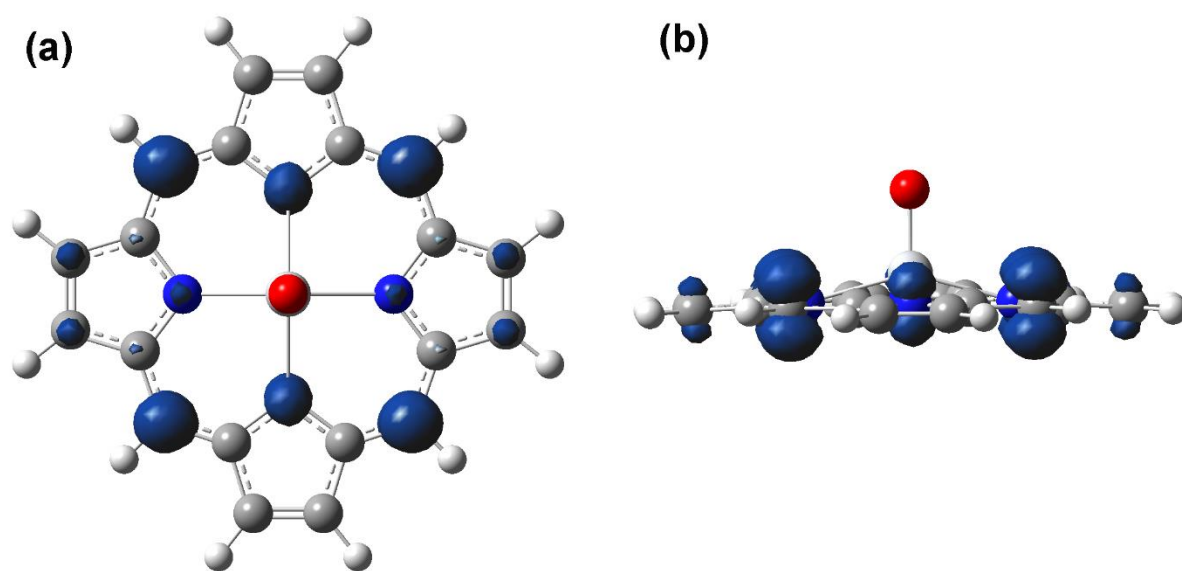


Figure S3. Spin density plot of triplet state TiO-Por.