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Electron and proton transfer reactions mediated by flavins in different molecular environments

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Publications

Papers related to this thesis

- The reorganization free energies for electron transfer in protein: Redox Properties of Flavin in BLUF and LOV Domains
M. Kılıç and B. Ensing
in preparation
- A microscopic picture of the solvent reorganization during electron transfer to flavin in water
M. Kılıç and B. Ensing
in preparation
- Acidity Constants of Lumiflavin from First Principles Molecular Simulation
M. Kılıç and B. Ensing
Phys. Chem. Chem. Phys. 16, 18993–19000, 2014.
- First and Second One-Electron Reduction of Lumiflavin in Water—A First Principles Molecular Dynamics Study
M. Kılıç and B. Ensing
J. Chem. Theory Comput. 9, 3889–3899, 2013.

Selected papers by the author

- Fe³⁺-doped TiO₂: A combined experimental and computational approach to the evaluation of visible light activity
Y. Yalçın, M. Kılıç and Z. Çımar
Appl. Catal. B Environ. 99, 469–477, 2010.
- Photocatalytic Degradation of Dinitronaphthalenes: Theory and Experiment
M. Bekbölet, Z. Çımar, M. Kılıç, C.S. Uyguner, C. Minero and E. Pelizzetti
Chemosphere 75, 1008–1014, 2009.
- Modeling of the Photocatalytic Degradation Reactions of Aromatic Pollutants: A Solvent Effect Model
M. Kılıç, N. San and Z. Çımar
J. Adv. Oxid. Technol. 10, 60–66, 2007.

- A Model for Prediction of Product Distributions for the Reactions of Phenol Derivatives with Hydroxyl Radicals
M. Kılıç, G. Koçtürk, N. San and Z. Çınar
Chemosphere 69, 1396–1408, 2007.