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### Molecular simulations in electrochemistry

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

Kılıç, M.

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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

- Fe<sup>3+</sup>-doped TiO<sub>2</sub>: 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.