

# Frédéric Labat

Born in Pau (France) — November 20, 1980

Current position: ATER  
LECIME – Msc – ENSCP  
11, rue Pierre et Marie Curie  
F-75231 Paris Cedex 05, France

☎ +33 1 44 27 67 28  
✉ [frederic-labat@enscp.fr](mailto:frederic-labat@enscp.fr)

## PAPERS IN PEER-REVIEWED JOURNALS

---

Referee for *the Journal of Physical Chemistry* and *Physical Chemistry Chemical Physics*.

[17] **F. Labat**, C. Pouchan, G.E. Scuseria and C. Adamo, “Performances of density functional theory for the description of two proton-ordered structures of ice”, in preparation

[16] **F. Labat**, I. Ciofini and C. Adamo, “Modeling the N<sub>3</sub>/TiO<sub>2</sub> interface in Dye-sensitized-solar cells using DFT”, *Chem. Mater.*, submitted

[15] T. Le Bahers, **F. Labat**, T. Pauporté and I. Ciofini, “Solvent and additives effects on the open circuit voltage of ZnO based Dye-sensitized-solar cells: a combined theoretical and experimental study”, *Phys. Chem. Chem. Phys.*, submitted

[14] T. Le Bahers, S. Di Tommaso, C. Peltier, G. Fayet, R. Giacomazzi, V. Tognetti, A. Prestianni, **F. Labat**, “Acridine orange in a pumpkin-shaped macrocycle: beyond solvent effects in the UV-visible spectra simulation of dyes”, *J. Mol. Struct.: Theochem*, in press, [doi:10.1016/j.theochem.2010.01.031](https://doi.org/10.1016/j.theochem.2010.01.031)

[13] **F. Labat**, A.H. Fuchs and C. Adamo, “Toward an Accurate Modeling of the Water-Zeolite Interaction: calibrating the DFT Approach”, *J. Phys. Chem. Lett.*, **1**, 763–768 (2010)

[12] **F. Labat**, I. Ciofini, H.P. Hratchian, M. Frisch, K. Raghavachari and C. Adamo, “First Principles Modeling of Eosin-Loaded ZnO Films: a Step toward the Understanding of Dye-Sensitized Solar Cell Performances”, *J. Am. Chem. Soc.*, **131**, 14290–14298 (2009)

[11] **F. Labat**, I. Ciofini and C. Adamo, “Modeling ZnO phases using a periodic approach: from bulk to surface and beyond”, *J. Chem. Phys.*, **131**, 044708–044719 (2009)

[10] **F. Labat** and C. Pouchan, “Adsorption of cyanodiacetylene on ice: a periodic approach”, *Phys. Chem. Chem. Phys.*, **11**, 5833–5842 (2009)

[9] A. Prestianni, A. Martorana, **F. Labat**, I. Ciofini and C. Adamo, “A DFT investigation of CO oxidation over neutral and cationic gold clusters”, *J. Mol. Struct. (Theochem)*, **903**, 34–40 (2009)

[8] A. Prestianni, A. Martorana, I. Ciofini, **F. Labat** and C. Adamo, “CO Oxidation on cationic gold clusters: a theoretical study”, *J. Phys. Chem. C*, **112**, 18061–18066 (2008)

[7] S. Hazebroucq, **F. Labat**, D. Lincot and C. Adamo, “Theoretical insights on the electronic properties of eosin Y, an organic dye for photovoltaic applications”, *J. Phys. Chem. A* **112**, 7264–7270 (2008)

[6] **F. Labat**, Ph. Baranek and C. Adamo, “Structural and electronic properties of selected rutile and anatase TiO<sub>2</sub> surfaces : an ab initio investigation”, *J. Chem. Theory Comput.* **4**, 341–352 (2008)

[5] M. Rekhis, **F. Labat**, O. Ouamerali, I. Ciofini and C. Adamo, “Theoretical Analysis of the Electronic Properties of N<sub>3</sub> Derivatives”, J. Phys. Chem. A **111**, 13106–13111 (2007)

[4] **F. Labat** and C. Adamo, “Bi-isonicotinic acid on anatase (101): insights from theory”, J. Phys. Chem. C **41**, 15034–15042 (2007)

[3] **F. Labat**, Ph. Baranek, C. Domain, C. Minot and C. Adamo, “Density functional theory analysis of the structural and electronic properties of TiO<sub>2</sub> rutile and anatase polytypes: performances of different exchange-correlation functionals”, J. Chem. Phys. **126**, 154703–154713 (2007)

[2] A. Prestianni, A. Martorana, **F. Labat**, I. Ciofini and C. Adamo, “Theoretical insights on O<sub>2</sub> and CO adsorption on neutral and positively charged gold clusters”, J. Phys. Chem. B **110**, 12240–12248 (2006)

[1] **F. Labat**, P.P. Lainé, I. Ciofini and C. Adamo, “Spectral properties of bipyridyl ligands by Time Dependent Density Functional Theory”, Chem. Phys. Lett. **417**, 445–451 (2005)