



Dr. Aurélie PERRIER

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Keywords: theoretical chemistry; quantum chemistry; molecular modeling; *ab initio* and DFT calculations; photoactive molecules; photochromic compounds; nanoparticles and nanoclusters.

Formation

- **2014** : Accreditation to supervise research (Habilitation à diriger les recherches, HDR), University Paris Diderot, France.
- **2005** : PhD in Physical Chemistry; University Bordeaux 1, France.
- **2002** : Master degree in theoretical chemistry, University Pierre et Marie Curie, France.
- **2002** : Chemical Engineer, Ecole Nationale Supérieure de Chimie de Paris (ENSCP), France.

Professional experience

- **2019-** : Associate Professor (HDR), Institute of Chemistry for Life and Health Sciences (FRE 2027), Université de Paris, France.
- **2014-2018** : Associate Professor (HDR), Institut de Recherche de Chimie Paris (UMR 8247) University Paris Diderot, France.
- **2007-2014** : Assistant Professor, ITODYS laboratory (UMR 7086), University Paris Diderot, France.
- **2006** : Post-doctoral researcher, Università degli studi di Siena, Siena, Italy.
- **2005** : Assistant Professor, Temporary position (ATER), University Paris Diderot, France.

Research activities

- Simulation of the structural and optical properties of photoactive molecules : photochromic molecules and charge-transfer systems.
- Simulation of the reactivity and photoreactivity of organic molecules.
- Simulation of the structural, redox and optical properties of metallic nanoparticles.
- Modeling of the interaction between redox probes (organometallic compounds) and biomolecules.

Supervision and administrative activities

- Supervision: 10 Bachelor, 6 Master 1, 3 Master 2, 2 PhD, 2 post-docs.
- Head of the Master 1 degree in Chemistry, Master 1 Chimie Paris Cité, Université de Paris.
- Member of the board of the Réseau Français de Chimie Théorique (RFCT), in charge of the communication.
- Member of the National Council of Universities (Conseil National des Universités, CNU), 2016-

Publications

Researcher ID : B-1525-2012 ; 61 articles ; h-index : 18 (01/01/19).

- Fihey, A; Maurel, F.; Perrier, A. Plasmon-exciton coupling for dithienylethenes/Gold nanoparticle hybrid systems *J. Phys. Chem. C* **2015**, *119*, 9995–10006.
- Fihey, A; Perrier, A.; Browne, W. R.; Jacquemin, D. Multiphotochromic molecular systems, *Chem. Soc. Rev.* **2015**, *44*, 3719–3759.
- Le Bras, L.; Adamo, C.; Perrier, A. Modeling the Modulation of Emission Behavior in E/Z Isomers of Dipyrrolyldiphenylethene: From Molecules to Nanoaggregates *J. Phys. Chem. C* **2017**, *45*, 25603–25616.
- Le Bras, L.; Chaitou, K.; ALoise, S.; Adamo, C.; Perrier, A. Aggregation-caused quenching versus crystallization induced emission in thiazolo[5,4-b]thieno[3,2-e]pyridine (TTP) derivatives: theoretical insights . *Phys. Chem. Chem. Phys.* **2019**, *2*, 46–56 .