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RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Chemistry, Physical Chemistry and Chemical Engineering
Subfield: Chemistry
Title: Better understanding TiO_2 photocatalysis by Density Functional Theory approaches

ParisTech School: Chimie ParisTech
Advisor(s) Name: Frédéric Labat
Advisor(s) Email: *frederic.labat@chimieparistech.psl.eu*
Research group/Lab: Theoretical Chemistry and Modeling Group/i-CLeHS FRE 2027 CNRS
(Lab/Advisor website): www.quanthic.fr

Short description of possible research topics for a PhD:
Photocatalysis, where solar energy is used to drive chemical and energy processes, has received considerable attention since it is a potentially environmentally friendly energy technology, with various applications in different fields such as solar cells, water splitting and pollutant degradation. In particular, heterogeneous photocatalysis, in which the catalyst is in a different phase as the reactants, has seen considerable developments, not only to propose new photocatalysts but also to better understand and improve photocatalytic processes.
Among the different photocatalysts proposed, TiO_2 is particularly appealing since it is chemically stable, nontoxic and low-cost. Although TiO_2-based heterogeneous photocatalysis has been successful during the last years, a clear understanding of the various processes involved during a typical photocatalytic reaction in TiO_2-based photocatalysis is however still largely missing, preventing a more rational design of new photocatalysts or the detailed characterization of new photocatalytic processes.
The aim of this project is to better understand, from a modeling viewpoint, basic processes involved in TiO_2-based heterogeneous photocatalysis, and how these processes influence the whole photocatalytic reaction. Particular care will be devoted to the development of cost effective computational approaches enabling the description of both ground and excited state properties of complex interfaces using both periodic ab-initio approaches rooted on Density Functional Theory and finite cluster models in conjunction with embedding techniques and implicit solvation models to simulate the effect of the environment.
Required background of the student: Physical Chemistry, Chemical Physics and, if possible, theoretical chemistry and previous programming experience.
A list of 5(max.) representative publications of the group:
[1] F. Labat et al "Silver-decorated CeO2 (111) as a potential anodic electrocatalyst in fuel cells: a hybrid Density Functional Theory investigation", *J. Phys. Chem. C*, **123**, 25668-25679 (2019).
[2] F. Labat, et al "Improving the Heterointerface in Hybrid Organic-Inorganic Perovskite Solar Cells by Surface Engineering: Insights from Periodic Hybrid Density Functional Theory Calculations", *J. Comput. Chem.*, **41**, 1740-1747 (2020).
[3] F. Labat et al , "On the stability issues of TiO2-based composites in view of fuel cell application: a combined experimental and theoretical investigation", *J. Phys. Chem. C*, **123**, 12573–12582 (2019).
[4] F. Labat, et al, "First-principles modeling of dye-sensitized solar cells: Challenges and perspectives", *Acc. Chem. Res.*, **45**, 1268 (2012).