FrÃ©dÃ©ric Labat

List of Publications by Year
in descending order

41 papers	1,839 citations	361413 20 h-index	265206 42 g-index
42 all docs	42 docs citations	42 times ranked	2530 citing authors

#	Article	IF	Citations
1	Density functional theory analysis of the structural and electronic properties of TiO2 rutile and anatase polytypes: Performances of different exchange-correlation functionals. Journal of Chemical Physics, 2007, 126, 154703.	3.0	307
2	Structural and Electronic Properties of Selected Rutile and Anatase TiO₂Surfaces:â€‰ An ab Initio Investigation. Journal of Chemical Theory and Computation, 2008, 4, 341-352.	5.3	204
3	First-Principles Modeling of Dye-Sensitized Solar Cells: Challenges and Perspectives. Accounts of Chemical Research, 2012, 45, 1268-1277.	15.6	194
4	First Principles Modeling of Eosin-Loaded ZnO Films: A Step toward the Understanding of Dye-Sensitized Solar Cell Performances. Journal of the American Chemical Society, 2009, 131, 14290-14298.	13.7	124
5	Modeling Dye-Sensitized Solar Cells: From Theory to Experiment. Journal of Physical Chemistry Letters, 2013, 4, 1044-1050.	4.6	104
6	Theoretical Procedure for Optimizing Dye-Sensitized Solar Cells: From Electronic Structure to Photovoltaic Efficiency. Journal of the American Chemical Society, 2011, 133, 8005-8013.	13.7	85
7	Revealing the Origins of Mechanically Induced Fluorescence Changes in Organic Molecular Crystals. Advanced Materials, 2018, 30, e1800817.	21.0	82
8	Insights into Working Principles of Ruthenium Polypyridyl Dye-Sensitized Solar Cells from First Principles Modeling. Journal of Physical Chemistry C, 2011, 115, 4297-4306.	3.1	71
9	A comprehensive DFT investigation of bulk and low-index surfaces of ZrO₂polymorphs. Journal of Computational Chemistry, 2015, 36, 9-21.	3.3	61
10	Electronic properties of PbX₃CH₃NH₃(X = Cl, Br, I) compounds for photovoltaic and photocatalytic applications. Physical Chemistry Chemical Physics, 2015, 17, 2199-2209.	2.8	52
11	Understanding Aggregation-Induced Emission in Molecular Crystals: Insights from Theory. Journal of Physical Chemistry C, 2017, 121, 5747-5752.	3.1	52
12	Interfacial Engineering through Chloride-Functionalized Self-Assembled Monolayers for High-Performance Perovskite Solar Cells. ACS Applied Materials & Interfaces, 2020, 12, 744-752.	8.0	47
13	Computational Protocol for Modeling Thermochromic Molecular Crystals: Salicylidene Aniline As a Case Study. Journal of Chemical Theory and Computation, 2014, 10, 5577-5585.	5.3	44
14	Modeling ZnO phases using a periodic approach: From bulk to surface and beyond. Journal of Chemical Physics, 2009, 131, 044708.	3.0	43
15	Bi-isonicotinic Acid on Anatase (101):â€‰ Insights from Theory. Journal of Physical Chemistry C, 2007, 111, 15034-15042.	3.1	42
16	Response Enhancement of Selfâ€Powered Visibleâ€Blind UV Photodetectors by Nanostructured Heterointerface Engineering. Advanced Functional Materials, 2019, 29, 1903981.	14.9	30
17	Electrostatic Embedding To Model the Impact of Environment on Photophysical Properties of Molecular Crystals: A Self-Consistent Charge Adjustment Procedure. Journal of Chemical Theory and Computation, 2016, 12, 3316-3324.	5.3	28
18	Revisiting the importance of dye binding mode in dye-sensitized solar cells: a periodic viewpoint. Journal of Materials Chemistry, 2012, 22, 12205.	6.7	26

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19	Modeling emission features of salicylidene aniline molecular crystals: A QM/QMâ€™ approach. Journal of Computational Chemistry, 2016, 37, 861-870.	3.3	26
20	Conduction Mechanisms in Oxideâ€“Carbonate Electrolytes for SOFC: Highlighting the Role of the Interface from First-Principles Modeling. Journal of Physical Chemistry C, 2018, 122, 10067-10077.	3.1	22
21	O₂ Activation over Ag-Decorated CeO₂(111) and TiO₂(110) Surfaces: A Theoretical Comparative Investigation. Journal of Physical Chemistry C, 2020, 124, 25917-25930.	3.1	19
22	Anchoring groups for dyes in p-DSSC application: insights from DFT. Journal of Molecular Modeling, 2016, 22, 289.	1.8	18
23	Mixed lithium-sodium (LiNaCO3) and lithium-potassium (LiKCO3) carbonates for low temperature electrochemical applications: Structure, electronic properties and surface reconstruction from ab-initio calculations. Surface Science, 2016, 647, 66-77.	1.9	18
24	Aggregation Effects on Pigment Coatings: Pigment Red 179 as a Case Study. ACS Omega, 2019, 4, 20315-20323.	3.5	18
25	Investigation of the bulk and surface properties of CdSe: insights from theory. Physical Chemistry Chemical Physics, 2014, 16, 23251-23259.	2.8	17
26	Optical properties of the dibenzothiazolylphenol molecular crystals through ONIOM calculations: the effect of the electrostatic embedding scheme. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	14
27	Assessing the performances of different continuum solvation models for the calculation of hydration energies of molecules, polymers and surfaces: a comparison between the SMD, VASPsol and FDPB models. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	13
28	Combined Computational and Experimental Study of CdSeS/ZnS Nanoplatelets: Structural, Vibrational, and Electronic Aspects of Coreâ€“Shell Interface Formation. Langmuir, 2018, 34, 13828-13836.	3.5	9
29	H₂ Dissociation and Water Evolution on Silver-Decorated CeO₂(111): A Hybrid Density Functional Theory Investigation. Journal of Physical Chemistry C, 2019, 123, 25668-25679.	3.1	9
30	Implicit Solvation Using a Generalized Finite-Difference Approach in CRYSTAL: Implementation and Results for Molecules, Polymers, and Surfaces. Journal of Chemical Theory and Computation, 2018, 14, 5969-5983.	5.3	8
31	Improving the heterointerface in hybrid organicâ€“inorganic perovskite solar cells by surface engineering: Insights from periodic hybrid density functional theory calculations. Journal of Computational Chemistry, 2020, 41, 1740-1747.	3.3	8
32	Defect Formation and Diffusion on the (001) Surface of LiKCO3 for Fuel Cell Applications: Insight from Hybrid DFT. Journal of Physical Chemistry C, 2016, 120, 12941-12951.	3.1	7
33	Analytical calculation of the solventâ€accessible surface area and its nuclear gradients by stereographic projection: A general approach for molecules, polymers, nanotubes, helices, and surfaces. Journal of Computational Chemistry, 2020, 41, 1464-1479.	3.3	7
34	Evaluation of the performances of different atomic charge and nonelectrostatic models in the finiteâ€difference <scp>Poissonâ€“Boltzmann</scp> approach. International Journal of Quantum Chemistry, 2021, 121, e26560.	2.0	7
35	Towards the modeling of quantum-dot sensitized solar cells: from structural and vibrational features to electron injection through lattice-mismatched interfaces. Journal of Materials Chemistry A, 2016, 4, 13081-13092.	10.3	4
36	Ex situ and in situ sensitized quantum dot solar cells. Physica Status Solidi (B): Basic Research, 2017, 254, 1600443.	1.5	3

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37	On the Stability Issues of TiO₂-Based Composites in View of Fuel Cell Application: A Combined Experimental and Theoretical Investigation. Journal of Physical Chemistry C, 2019, 123, 12573-12582.	3.1	3
38	Modeling UVâ€“Vis spectra of low dimensional materials using electrostatic embedding: The case of CdSe. Journal of Computational Chemistry, 2021, 42, 1212-1224.	3.3	3
39	Modeling the spectral properties of poly(xâ€phenylenediamine) conducting polymers using a combined <scp>TDâ€DFT</scp> and electrostatic embedding approach. Journal of Computational Chemistry, 2022, 43, 2001-2008.	3.3	3
40	Generalizing Continuum Solvation in Crystal to Nonaqueous Solvents: Implementation, Parametrization, and Application to Molecules and Surfaces. Journal of Chemical Theory and Computation, 2021, 17, 6432-6448.	5.3	2
41	Towards a transferable nonelectrostatic model for continuum solvation: The electrostatic and nonelectrostatic energy correction model. Journal of Computational Chemistry, 2022, 43, 1372-1387.	3.3	2