FrÃ©dÃ©ric Labat

List of Publications by Year
in descending order

41	1,839	361413	265206
papers	citations	20	42
		h-index	g-index

42	42	42	2530
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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
2	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
3	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
4	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
5	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
6	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
7	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
8	O_2 Activation over Ag-Decorated CeO_2(111) and TiO_2(110) Surfaces: A Theoretical Comparative Investigation. Journal of Physical Chemistry C, 2020, 124, 25917-25930.	3.1	19
9	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
10	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
11	Response Enhancement of Selfâ€Powered Visibleâ€Blind UV Photodetectors by Nanostructured Heterointerface Engineering. Advanced Functional Materials, 2019, 29, 1903981.	14.9	30
12	H_2 Dissociation and Water Evolution on Silver-Decorated CeO_2(111): A Hybrid Density Functional Theory Investigation. Journal of Physical Chemistry C, 2019, 123, 25668-25679.	3.1	9
13	On the Stability Issues of TiO_2-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
14	Aggregation Effects on Pigment Coatings: Pigment Red 179 as a Case Study. ACS Omega, 2019, 4, 20315-20323.	3.5	18
15	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
16	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
17	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
18	Revealing the Origins of Mechanically Induced Fluorescence Changes in Organic Molecular Crystals. Advanced Materials, 2018, 30, e1800817.	21.0	82

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19	Understanding Aggregation-Induced Emission in Molecular Crystals: Insights from Theory. Journal of Physical Chemistry C, 2017, 121, 5747-5752.	3.1	52
20	*Ex situ* and *in situ* sensitized quantum dot solar cells. Physica Status Solidi (B): Basic Research, 2017, 254, 1600443.	1.5	3
21	Modeling emission features of salicylidene aniline molecular crystals: A QM/QM′ approach. Journal of Computational Chemistry, 2016, 37, 861-870.	3.3	26
22	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
23	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
24	Anchoring groups for dyes in p-DSSC application: insights from DFT. Journal of Molecular Modeling, 2016, 22, 289.	1.8	18
25	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
26	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
27	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
28	Electronic properties of $PbX_3CH_3NH_3$ (X = Cl, Br, I) compounds for photovoltaic and photocatalytic applications. Physical Chemistry Chemical Physics, 2015, 17, 2199-2209.	2.8	52
29	A comprehensive DFT investigation of bulk and low-index surfaces of ZrO_2 polymorphs. Journal of Computational Chemistry, 2015, 36, 9-21.	3.3	61
30	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
31	Investigation of the bulk and surface properties of CdSe: insights from theory. Physical Chemistry Chemical Physics, 2014, 16, 23251-23259.	2.8	17
32	Modeling Dye-Sensitized Solar Cells: From Theory to Experiment. Journal of Physical Chemistry Letters, 2013, 4, 1044-1050.	4.6	104
33	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
34	First-Principles Modeling of Dye-Sensitized Solar Cells: Challenges and Perspectives. Accounts of Chemical Research, 2012, 45, 1268-1277.	15.6	194
35	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
36	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

#	Article	IF	Citations
37	Modeling ZnO phases using a periodic approach: From bulk to surface and beyond. Journal of Chemical Physics, 2009, 131, 044708.	3.0	43
38	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
39	Structural and Electronic Properties of Selected Rutile and Anatase TiO$_2$ Surfaces:â€‰ An ab Initio Investigation. Journal of Chemical Theory and Computation, 2008, 4, 341-352.	5.3	204
40	Bi-isonicotinic Acid on Anatase (101):â€‰ Insights from Theory. Journal of Physical Chemistry C, 2007, 111, 15034-15042.	3.1	42
41	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