Gianluca Levi

List of Publications by Year in Descending Order

26 papers	304 citations	10 h-index	17 g-index
27 ext. papers	362 ext. citations	2.7 avg, IF	3.75 L-index

#	Paper	IF	Citations
26	Variational Density Functional Calculations of Excited States: Conical Intersection and Avoided Crossing in Ethylene Bond Twisting.. *Journal of Physical Chemistry Letters*, **2022**, 3990-3999	6.4	2
25	Method for Calculating Excited Electronic States Using Density Functionals and Direct Orbital Optimization with Real Space Grid or Plane-Wave Basis Set. *Journal of Chemical Theory and Computation*, **2021**, 17, 5034-5049	6.4	5
24	On how mild oxidation affects the structure of carbons: Comparative analysis by different techniques. *Applications in Energy and Combustion Science*, **2020**, 1-4, 100006	0.8	1
23	Variational calculations of excited states direct optimization of the orbitals in DFT. *Faraday Discussions*, **2020**, 224, 448-466	3.6	19
22	On the interplay of solvent and conformational effects in simulated excited-state dynamics of a copper phenanthroline photosensitizer. *Physical Chemistry Chemical Physics*, **2020**, 22, 748-757	3.6	16
21	Variational Density Functional Calculations of Excited States via Direct Optimization. *Journal of Chemical Theory and Computation*, **2020**, 16, 6968-6982	6.4	25
20	New approaches to study excited states in density functional theory: general discussion. *Faraday Discussions*, **2020**, 224, 483-508	3.6	2
19	Excited-state solvation structure of transition metal complexes from molecular dynamics simulations and assessment of partial atomic charge methods. *Physical Chemistry Chemical Physics*, **2019**, 21, 4082-4095	3.6	8
18	Dynamics of Excited-State Bond Formation. *Springer Theses*, **2019**, 165-186	0.1	
17	The Diplatinum Complex PtPOP. *Springer Theses*, **2019**, 13-17	0.1	
16	Equilibrium Solution Structure. *Springer Theses*, **2019**, 143-155	0.1	
15	Coherent Vibrational Dynamics in the Ground State. *Springer Theses*, **2019**, 157-163	0.1	
14	Simulating and Analysing X-Ray Diffuse Scattering Signals. *Springer Theses*, **2019**, 99-107	0.1	
13	Filming Motion at the Atomic Scale of Time. *Springer Theses*, **2019**, 3-11	0.1	
12	Computational Details of the QM/MM BOMD Simulations. *Springer Theses*, **2019**, 125-141	0.1	
11	Observing Molecular Motion in Solution with X-Rays. *Springer Theses*, **2019**, 89-97	0.1	
10	Density Functional Methods. *Springer Theses*, **2019**, 29-70	0.1	

9	The Quantum Mechanics/Molecular Mechanics Method. *Springer Theses*, **2019**, 71-86	0.1	
8	Gas-Phase Molecular Geometry. *Springer Theses*, **2019**, 111-123	0.1	
7	Ultrafast X-Ray Scattering Measurements of Coherent Structural Dynamics on the Ground-State Potential Energy Surface of a Diplatinum Molecule. *Physical Review Letters*, **2019**, 122, 063001	7.4	41
6	Theoretical Evidence of Solvent-Mediated Excited-State Dynamics in a Functionalized Iron Sensitizer. *Journal of Physical Chemistry C*, **2019**, 123, 2056-2065	3.8	18
5	Solution Structure and Ultrafast Vibrational Relaxation of the PtPOP Complex Revealed by SCF-QM/MM Direct Dynamics Simulations. *Journal of Physical Chemistry C*, **2018**, 122, 7100-7119	3.8	35
4	Anisotropy enhanced X-ray scattering from solvated transition metal complexes. *Journal of Synchrotron Radiation*, **2018**, 25, 306-315	2.4	26
3	Mechanism and Thermochemistry of Coal Char Oxidation and Desorption of Surface Oxides. *Energy & Fuels*, **2017**, 31, 2308-2316	4.1	10
2	Grid-Based Projector Augmented Wave (GPAW) Implementation of Quantum Mechanics/Molecular Mechanics (QM/MM) Electrostatic Embedding and Application to a Solvated Diplatinum Complex. *Journal of Chemical Theory and Computation*, **2017**, 13, 6010-6022	6.4	24
1	Probing the chemical nature of surface oxides during coal char oxidation by high-resolution XPS. *Carbon*, **2015**, 90, 181-196	10.4	72