Gianluca Levi

List of Publications by Year
in descending order

25	443	840119 11	1058022 14
papers	citations	h-index	g-index

27	27	27	621
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Probing the chemical nature of surface oxides during coal char oxidation by high-resolution XPS. Carbon, 2015, 90, 181-196.	5.4	88
2	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.	2.9	64
3	Solution Structure and Ultrafast Vibrational Relaxation of the PtPOP Complex Revealed by Î"SCF-QM/MM Direct Dynamics Simulations. Journal of Physical Chemistry C, 2018, 122, 7100-7119.	1.5	46
4	Variational Density Functional Calculations of Excited States via Direct Optimization. Journal of Chemical Theory and Computation, 2020, 16, 6968-6982.	2.3	45
5	Anisotropy enhanced X-ray scattering from solvated transition metal complexes. Journal of Synchrotron Radiation, 2018, 25, 306-315.	1.0	33
6	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.	2.3	32
7	Variational calculations of excited states via direct optimization of the orbitals in DFT. Faraday Discussions, 2020, 224, 448-466.	1.6	31
8	Theoretical Evidence of Solvent-Mediated Excited-State Dynamics in a Functionalized Iron Sensitizer. Journal of Physical Chemistry C, 2019, 123, 2056-2065.	1.5	29
9	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.	1.3	25
10	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.	1.3	15
11	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.	2.3	12
12	Mechanism and Thermochemistry of Coal Char Oxidation and Desorption of Surface Oxides. Energy & Fuels, 2017, 31, 2308-2316.	2.5	11
13	Variational Density Functional Calculations of Excited States: Conical Intersection and Avoided Crossing in Ethylene Bond Twisting. Journal of Physical Chemistry Letters, 2022, 13, 3990-3999.	2.1	9
14	New approaches to study excited states in density functional theory: general discussion. Faraday Discussions, 2020, 224, 483-508.	1.6	2
15	On how mild oxidation affects the structure of carbons: Comparative analysis by different techniques. Applications in Energy and Combustion Science, 2020, 1-4, 100006.	0.9	1
16	Dynamics of Excited-State Bond Formation. Springer Theses, 2019, , 165-186.	0.0	0
17	The Diplatinum Complex PtPOP. Springer Theses, 2019, , 13-17.	0.0	0
18	Equilibrium Solution Structure. Springer Theses, 2019, , 143-155.	0.0	0

#	Article	IF	Citations
19	Coherent Vibrational Dynamics in the Ground State. Springer Theses, 2019, , 157-163.	0.0	0
20	Simulating and Analysing X-Ray Diffuse Scattering Signals. Springer Theses, 2019, , 99-107.	0.0	0
21	Filming Motion at the Atomic Scale of Time. Springer Theses, 2019, , 3-11.	0.0	0
22	Observing Molecular Motion in Solution with X-Rays. Springer Theses, 2019, , 89-97.	0.0	0
23	Density Functional Methods. Springer Theses, 2019, , 29-70.	0.0	0
24	The Quantum Mechanics/Molecular Mechanics Method. Springer Theses, 2019, , 71-86.	0.0	0
25	Gas-Phase Molecular Geometry. Springer Theses, 2019, , 111-123.	0.0	0