Lara Ferrighi

List of Publications by Year
in descending order

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46 papers	4,500 citations	201674 27 h-index	233421 45 g-index
46 all docs	46 docs citations	46 times ranked	6700 citing authors

#	Article	IF	Citations
1	Electronic structure calculations with GPAW: a real-space implementation of the projector augmented-wave method. Journal of Physics Condensed Matter, 2010, 22, 253202.	1.8	1,451
2	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	14.6	1,166
3	Single and Multiple Doping in Graphene Quantum Dots: Unraveling the Origin of Selectivity in the Oxygen Reduction Reaction. ACS Catalysis, 2015, 5, 129-144.	11.2	166
4	Boron-doped graphene as active electrocatalyst for oxygen reduction reaction at a fuel-cell cathode. Journal of Catalysis, 2014, 318, 203-210.	6.2	134
5	2Dâ”3D Transition for Cationic and Anionic Gold Clusters: A Kinetic Energy Density Functional Study. Journal of the American Chemical Society, 2009, 131, 10605-10609.	13.7	124
6	Density-functional-theory study of the electric-field-induced second harmonic generation (EFISHG) of pushâ€“pull phenylpolyenes in solution. Chemical Physics Letters, 2006, 425, 267-272.	2.6	99
7	Direct Observation of Molecular Preorganization for Chirality Transfer on a Catalyst Surface. Science, 2011, 334, 776-780.	12.6	84
8	Boosting Graphene Reactivity with Oxygen by Boron Doping: Density Functional Theory Modeling of the Reaction Path.. Journal of Physical Chemistry C, 2014, 118, 223-230.	3.1	78
9	Density functional theory based screening of ternary alkali-transition metal borohydrides: A computational material design project. Journal of Chemical Physics, 2009, 131, 014101.	3.0	77
10	Catalysis under Cover: Enhanced Reactivity at the Interface between (Doped) Graphene and Anatase TiO₂. Journal of the American Chemical Society, 2016, 138, 7365-7376.	13.7	69
11	Solvent effects on two-photon absorption of dialkylamino substituted distyrylbenzene chromophore. Journal of Chemical Physics, 2007, 126, 204509.	3.0	68
12	Second-Harmonic Generation in GFP-like Proteins. Journal of the American Chemical Society, 2008, 130, 15713-15719.	13.7	66
13	On-surface photo-dissociation of Câ€“Br bonds: towards room temperature Ullmann coupling. Chemical Communications, 2015, 51, 12593-12596.	4.1	66
14	Boron-Doped, Nitrogen-Doped, and Codoped Graphene on Cu(111): A DFT + vdW Study. Journal of Physical Chemistry C, 2015, 119, 6056-6064.	3.1	63
15	Spherical versus Faceted Anatase TiO₂ Nanoparticles: A Model Study of Structural and Electronic Properties. Journal of Physical Chemistry C, 2015, 119, 20735-20746.	3.1	58
16	Treatment of Layered Structures Using a Semilocal meta-GGA Density Functional. Journal of Physical Chemistry Letters, 2010, 1, 515-519.	4.6	55
17	Interaction between Coronene and Graphite from Temperature-Programmed Desorption and DFT-vdW Calculations: Importance of Entropic Effects and Insights into Graphite Interlayer Binding. Journal of Physical Chemistry C, 2013, 117, 13520-13529.	3.1	45
18	Study of Alkylthiolate Self-assembled Monolayers on Au(111) Using a Semilocal meta-GGA Density Functional. Journal of Physical Chemistry C, 2012, 116, 7374-7379.	3.1	43

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19	Second-harmonic generation of solvated molecules using multiconfigurational self-consistent-field quadratic response theory and the polarizable continuum model. Journal of Chemical Physics, 2005, 123, 144117.	3.0	42
20	Self-consistent meta-generalized gradient approximation study of adsorption of aromatic molecules on noble metal surfaces. Journal of Chemical Physics, 2011, 135, 084704.	3.0	38
21	Stereodirection of an Î±-Ketoester at Sub-molecular Sites on Chirally Modified Pt(111): Heterogeneous Asymmetric Catalysis. Journal of the American Chemical Society, 2013, 135, 9999-10002.	13.7	37
22	Charge Carriers Separation at the Graphene/(101) Anatase TiO₂ Interface. Advanced Materials Interfaces, 2016, 3, 1500624.	3.7	37
23	Photoexcited carriers recombination and trapping in spherical vs faceted TiO2 nanoparticles. Nano Energy, 2016, 27, 673-689.	16.0	37
24	Solvent effects on the conformational distribution and optical rotation of Î³-methyl paraconic acids and esters. Chirality, 2006, 18, 357-369.	2.6	32
25	Two-photon absorption of [2.2]paracyclophane derivatives in solution: A theoretical investigation. Journal of Chemical Physics, 2007, 127, 244103.	3.0	32
26	Ab initio n-electron valence state perturbation theory study of the adiabatic transitions in carbonyl molecules: Formaldehyde, acetaldehyde, and acetone. Journal of Chemical Physics, 2005, 122, 114304.	3.0	30
27	Control of the Intermolecular Coupling of Dibromotetracene on Cu(110) by the Sequential Activation of Cï£¿Br and Cï£¿H Bonds. Chemistry - A European Journal, 2015, 21, 5826-5835.	3.3	30
28	Surface-Confined Polymerization of Halogenated Polyacenes: The Case of Dibromotetracene on Ag(110). Journal of Physical Chemistry C, 2016, 120, 4909-4918.	3.1	29
29	Computational electrochemistry of doped graphene as electrocatalytic material in fuel cells. International Journal of Quantum Chemistry, 2016, 116, 1623-1640.	2.0	28
30	Water at the Interface Between Defective Graphene and Cu or Pt (111) Surfaces. ACS Applied Materials & Interfaces, 2017, 9, 29932-29941.	8.0	22
31	Synthesis of graphene nanoribbons with a defined mixed edge-site sequence by surface assisted polymerization of (1,6)-dibromopyrene on Ag(110). Nanoscale, 2016, 8, 17843-17853.	5.6	20
32	Analytic ab initio calculations of coherent anti-Stokes Raman scattering (CARS). Physical Chemistry Chemical Physics, 2009, 11, 2293.	2.8	19
33	A CASSCF theoretical study of the vibrational frequencies and structure of formaldehyde, acetaldehyde and acetone valence excited states. Computational and Theoretical Chemistry, 2005, 718, 55-69.	1.5	18
34	Alkane dimers interaction: A semi-local MGGA functional study. Chemical Physics Letters, 2010, 492, 183-186.	2.6	17
35	Ï€ Magnetism of Carbon Monovacancy in Graphene by Hybrid Density Functional Calculations. Journal of Physical Chemistry C, 2017, 121, 8653-8661.	3.1	17
36	Oxygen reactivity on pure and B-doped graphene over crystalline Cu(111). Effects of the dopant and of the metal support. Surface Science, 2015, 634, 68-75.	1.9	16

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37	Degenerate Four-Wave Mixing in Solution by Cubic Response Theory and the Polarizable Continuum Model. Journal of Physical Chemistry B, 2007, 111, 8965-8973.	2.6	15
38	Solvent Effects on the Three-Photon Absorption of a Symmetric Charge-Transfer Molecule. Journal of Physical Chemistry B, 2008, 112, 4703-4710.	2.6	15
39	Developments in then-electron valence state perturbation theory. International Journal of Quantum Chemistry, 2006, 106, 686-691.	2.0	13
40	Theoretical Studies of Oxygen Reactivity of Freeâ€Standing and Supported Boronâ€Doped Graphene. ChemSusChem, 2016, 9, 1061-1077.	6.8	12
41	Parallelization of the integral equation formulation of the polarizable continuum model for higher-order response functions. Journal of Chemical Physics, 2006, 125, 154112.	3.0	10
42	Synthesis of corrugated C-based nanostructures by Br-corannulene oligomerization. Physical Chemistry Chemical Physics, 2018, 20, 26161-26172.	2.8	9
43	Excited-state polarizabilities of solvated molecules using cubic response theory and the polarizable continuum model. Journal of Chemical Physics, 2010, 132, 024107.	3.0	8
44	Gauge-origin-independent magnetizabilities of solvated molecules using the polarizable continuum model. Journal of Chemical Physics, 2005, 123, 204104.	3.0	4
45	The Norwegian National Ground Segment; Preservation, Distribution and Exploitation of Sentinel Data. Data Science Journal, 2019, 18, .	1.3	1
46	Keeping Track of Samples in Multidisciplinary Fieldwork. Data Science Journal, 2021, 20, .	1.3	0