Veronica Barone

List of Publications by Year
in descending order

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63	6,739	147566	133063
papers	citations	31 h-index	59 g-index

64	64	64	8679
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Gas processing with intrinsically porous 2D membranes. Materials Chemistry and Physics, 2022, 276, 125426.	2.0	2
2	Structural and electronic properties of layered nanoporous organic nanocrystals. RSC Advances, 2021, 11, 5773-5784.	1.7	4
3	Machine Learning Screening of Metal-Ion Battery Electrode Materials. ACS Applied Materials & Interfaces, 2021, 13, 53355-53362.	4.0	42
4	Computational Study of Ortho-Substituent Effects on Antioxidant Activities of Phenolic Dendritic Antioxidants. Antioxidants, 2020, 9, 189.	2.2	41
5	Thickness dependence of solar cell efficiency in transition metal dichalcogenides MX2 (M: Mo, W; X: S,) Tj ETQq1 1 0.784314 rgBT /O	3.0	19
6	Structure and stability of graphene-like layers built from heterocyclic units. Carbon, 2019, 152, 128-133.	5.4	10
7	Machine Learning the Voltage of Electrode Materials in Metal-Ion Batteries. ACS Applied Materials & Interfaces, 2019, 11, 18494-18503.	4.0	104
8	Voltage stabilization of Sn-doped anatase for Li-ion battery applications predicted by DFT calculations. Materials Chemistry and Physics, 2019, 227, 347-351.	2.0	2
9	What is the maximum electrochemical Li insertion capacity in anatase? Insights from Density Functional Theory. Computational Materials Science, 2018, 152, 337-340.	1.4	2
10	Modeling of Quasi-One-Dimensional Carbon Nanostructures with Density Functional Theory. , 2017, , 1297-1337.		0
11	Two-dimensional nitrogen-rich transition metal compounds: The case of TiN 2. Journal of Electron Spectroscopy and Related Phenomena, 2017, 219, 29-34.	0.8	3
12	Tunable Broadband Nanocarbon Transparent Conductor by Electrochemical Intercalation. ACS Nano, 2017, 11, 788-796.	7.3	31
13	Comparison of oxidized carbon nanotubes for Li-ion storage capacity. Journal of Applied Electrochemistry, 2015, 45, 161-167.	1.5	4
14	Hexagonal BC₃: A Robust Electrode Material for Li, Na, and K Ion Batteries. Journal of Physical Chemistry Letters, 2015, 6, 2728-2732.	2.1	100
15	Potassium Ion Batteries with Graphitic Materials. Nano Letters, 2015, 15, 7671-7677.	4.5	805
16	Structural and electronic properties of crystalline graphite-like BC3. Computational Materials Science, 2015, 109, 248-252.	1.4	11
17	Gradient copolymers of thiophene and pyrrole for photovoltaics. Computational Materials Science, 2015, 96, 69-71.	1.4	7
18	Modeling of Quasi-One-Dimensional Carbon Nanostructures with Density Functional Theory. , 2015, , 1-41.		0

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19	Li adsorption on edge-oxidized graphene nanoribbons predicted by DFT calculations. Surface Science, 2014, 619, 105-113.	0.8	24
20	Scalable Holey Graphene Synthesis and Dense Electrode Fabrication toward High-Performance Ultracapacitors. ACS Nano, 2014, 8, 8255-8265.	7.3	212
21	Site-specific polarizabilities from analytic linear-response theory. Chemical Physics Letters, 2014, 608, 24-27.	1.2	0
22	Accurate Surface Chemistry beyond the Generalized Gradient Approximation: Illustrations for Graphene Adatoms. Journal of Chemical Theory and Computation, 2013, 9, 4853-4859.	2.3	20
23	On the chemical nature of thermally reduced graphene oxide and its electrochemical Li intake capacity. Carbon, 2013, 61, 558-567.	5.4	46
24	Synthesis, characterization, and DFT study of polycyclic aromatic hydrocarbon precursors, 1,4-diiodo-2,3,5,6-tetraarylbenzene and 1,4-bis(4-bromophenyl)-2,3,5,6-tetraarylbenzene. Journal of Molecular Structure, 2013, 1032, 41-47.	1.8	4
25	Lithium Adsorption on Graphene: From Isolated Adatoms to Metallic Sheets. Journal of Chemical Theory and Computation, 2012, 8, 1064-1071.	2.3	79
26	Modeling of Quasi-One-Dimensional Carbon Nanostructures with Density Functional Theory. , 2012, , 901-938.		2
27	Synthesis, characterization and DFT study of 1-bromo-4-(3,7-dimethyloctyl)benzene. Journal of Molecular Structure, 2012, 1015, 41-45.	1.8	3
28	Accurate Prediction of the Electronic Properties of Low-Dimensional Graphene Derivatives Using a Screened Hybrid Density Functional. Accounts of Chemical Research, 2011, 44, 269-279.	7.6	115
29	Enhanced Electrochemical Lithium Storage by Graphene Nanoribbons. Journal of the American Chemical Society, 2010, 132, 12556-12558.	6.6	259
30	Electronic Properties of the Biphenylene Sheet and Its One-Dimensional Derivatives. ACS Nano, 2010, 4, 4565-4570.	7.3	124
31	Edge Effects on the Characteristics of Li Diffusion in Graphene. Nano Letters, 2010, 10, 2838-2842.	4.5	428
32	Lithium adsorption on zigzag graphene nanoribbons. Journal of Applied Physics, 2009, 106, .	1.1	117
33	Magnetic exchange couplings from noncollinear spin density functional perturbation theory. Journal of Chemical Physics, 2008, 129, 194107.	1.2	24
34	Half-metallic graphene nanodots: A comprehensive first-principles theoretical study. Physical Review B, 2008, 77, .	1.1	290
35	Accurate solid-state band gaps via screened hybrid electronic structure calculations. Journal of Chemical Physics, 2008, 129, 011102.	1.2	147
36	Magnetic Boron Nitride Nanoribbons with Tunable Electronic Properties. Nano Letters, 2008, 8, 2210-2214.	4.5	317

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37	Enhanced Half-Metallicity in Edge-Oxidized Zigzag Graphene Nanoribbons. Nano Letters, 2007, 7, 2295-2299.	4.5	547
38	Energy storage capacity of polymeric nitrogen. Molecular Physics, 2006, 104, 745-749.	0.8	42
39	Screened exchange hybrid density-functional study of the work function of pristine and doped single-walled carbon nanotubes. Journal of Chemical Physics, 2006, 124, 024709.	1.2	87
40	Theoretical Nitrogen NMR Chemical Shifts in Octahedral Boron Nitride Cages. Journal of Physical Chemistry A, 2006, 110, 10844-10847.	1.1	26
41	Electronic Structure and Stability of Semiconducting Graphene Nanoribbons. Nano Letters, 2006, 6, 2748-2754.	4.5	1,568
42	Theoretical NMR nJ(13C,13C) Scalar Couplings as Probes to Study Diamagnetic Ring Currents in Fullerenes. Advances in Quantum Chemistry, 2005, , 127-139.	0.4	3
43	Prediction of vicinal protonâ€“proton coupling constants³J_{HH}from density functional theory calculations. Molecular Physics, 2005, 103, 1307-1326.	0.8	16
44	Optical Transitions in Metallic Single-Walled Carbon Nanotubes. Nano Letters, 2005, 5, 1830-1833.	4.5	66
45	Density Functional Theory Study of Optical Transitions in Semiconducting Single-Walled Carbon Nanotubes. Nano Letters, 2005, 5, 1621-1624.	4.5	92
46	Assessment of Density Functionals for Predicting One-Bond Carbonâ^'Hydrogen NMR Spinâ^'Spin Coupling Constants. Journal of Chemical Theory and Computation, 2005, 1, 541-545.	2.3	66
47	Theoretical study of the electronic properties of narrow single-walled carbon nanotubes: Beyond the local density approximation. Journal of Chemical Physics, 2004, 121, 10376-10379.	1.2	53
48	Substituent effects on scalarJ(13C,13C) couplings in pyrimidines. An experimental and DFT study. Magnetic Resonance in Chemistry, 2004, 42, 938-943.	1.1	5
49	Effect of oxygen chemisorption on the energy band gap of a chiral semiconducting single-walled carbon nanotube. Chemical Physics Letters, 2004, 389, 289-292.	1.2	53
50	Interaction of atomic hydrogen with single-walled carbon nanotubes: A density functional theory study. Journal of Chemical Physics, 2004, 120, 7169-7173.	1.2	44
51	Density Functional Theory Calculation of Indirect Nuclear Magnetic Resonance Spinâ^'Spin Coupling Constants in C70. Journal of the American Chemical Society, 2004, 126, 7428-7429.	6.6	26
52	Substituent Effects on Scalar 2J(19F,19F) and 3J(19F,19F) NMR Couplings:â€‰ A Comparison of SOPPA and DFT Methods. Journal of Physical Chemistry A, 2003, 107, 4748-4754.	1.1	103
53	The spinâ€”orbit/Fermi contact effect on13C substituent chemical shifts in 1-halo-bicyclo[1.1.1]pentanes. Molecular Physics, 2003, 101, 1297-1301.	0.8	5
54	Advances in Theoretical and Physical Aspects of Spinâ€“Spin Coupling Constants. Annual Reports on NMR Spectroscopy, 2003, 51, 167-260.	0.7	102

#	Article	IF	Citations
55	Solvent Effects on Nuclear Magnetic Resonance 2J(C,Hf) and 1J(C,Hf) Spinâ€“Spin Coupling Constants in Acetaldehyde. International Journal of Molecular Sciences, 2003, 4, 93-106.	1.8	21
56	NaturalJcoupling (NJC) analysis of the electron lone pair effect on NMR couplings: 2. The anomeric effects on1J(C, H) couplings and its dependence on solvent. Molecular Physics, 2002, 100, 705-715.	0.8	32
57	On the Capriciousness of the FCCF Karplus Curve. Journal of the American Chemical Society, 2002, 124, 9702-9703.	6.6	25
58	DFT Calculation of NMRJFFSpinâ^'Spin Coupling Constants in Fluorinated Pyridines. Journal of Physical Chemistry A, 2002, 106, 5607-5612.	1.1	146
59	Finite perturbation theory-density functional theory calculation of the spin-dipolar contribution to NMR spin-spin coupling constants. Molecular Physics, 2001, 99, 655-661.	0.8	26
60	Through-Bond and Through-SpaceJFFSpinâ^'Spin Coupling in Peridifluoronaphthalenes:Â Accurate DFT Evaluation of the Four Contributions. Journal of the American Chemical Society, 2001, 123, 9162-9163.	6.6	88
61	Vicinal NMR Protonâ^'Proton Coupling Constants. An NBO Analysis. Journal of Physical Chemistry A, 2001, 105, 5298-5303.	1.1	25
62	NaturalJ coupling (NJC) analysis of the electron lone pair effect on NMR couplings: Part 1. The lone pair orientation effect of an ?-nitrogen atom on1J(C,C) couplings. Magnetic Resonance in Chemistry, 2001, 39, 600-606.	1.1	54
63	NMR3J(C1,H3) couplings in 1-X-bicyclo[1.1.1]pentanes. FPT-DFT and NBO studies of hyperconjugative interactions and heavy atom substituent effects. Journal of Computational Chemistry, 2001, 22, 1615-1621.	1.5	20