

# Veronica Barone

## List of Publications by Year in descending order

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63  
papers

6,739  
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147566

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all docs

64  
docs citations

64  
times ranked

8679  
citing authors

#	ARTICLE	IF	CITATIONS
1	Electronic Structure and Stability of Semiconducting Graphene Nanoribbons. Nano Letters, 2006, 6, 2748-2754.	4.5	1,568
2	Potassium Ion Batteries with Graphitic Materials. Nano Letters, 2015, 15, 7671-7677.	4.5	805
3	Enhanced Half-Metallicity in Edge-Oxidized Zigzag Graphene Nanoribbons. Nano Letters, 2007, 7, 2295-2299.	4.5	547
4	Edge Effects on the Characteristics of Li Diffusion in Graphene. Nano Letters, 2010, 10, 2838-2842.	4.5	428
5	Magnetic Boron Nitride Nanoribbons with Tunable Electronic Properties. Nano Letters, 2008, 8, 2210-2214.	4.5	317
6	Half-metallic graphene nanodots: A comprehensive first-principles theoretical study. Physical Review B, 2008, 77, .	1.1	290
7	Enhanced Electrochemical Lithium Storage by Graphene Nanoribbons. Journal of the American Chemical Society, 2010, 132, 12556-12558.	6.6	259
8	Scalable Holey Graphene Synthesis and Dense Electrode Fabrication toward High-Performance Ultracapacitors. ACS Nano, 2014, 8, 8255-8265.	7.3	212
9	Accurate solid-state band gaps via screened hybrid electronic structure calculations. Journal of Chemical Physics, 2008, 129, 011102.	1.2	147
10	DFT Calculation of NMR JFFSpin <sup>~</sup> Spin Coupling Constants in Fluorinated Pyridines. Journal of Physical Chemistry A, 2002, 106, 5607-5612.	1.1	146
11	Electronic Properties of the Biphenylene Sheet and Its One-Dimensional Derivatives. ACS Nano, 2010, 4, 4565-4570.	7.3	124
12	Lithium adsorption on zigzag graphene nanoribbons. Journal of Applied Physics, 2009, 106, .	1.1	117
13	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
14	Machine Learning the Voltage of Electrode Materials in Metal-Ion Batteries. ACS Applied Materials & Interfaces, 2019, 11, 18494-18503.	4.0	104
15	Substituent Effects on Scalar $2J(19F,19F)$ and $3J(19F,19F)$ NMR Couplings: A Comparison of SOPPA and DFT Methods. Journal of Physical Chemistry A, 2003, 107, 4748-4754.	1.1	103
16	Advances in Theoretical and Physical Aspects of Spin <sup>~</sup> Spin Coupling Constants. Annual Reports on NMR Spectroscopy, 2003, 51, 167-260.	0.7	102
17	Hexagonal BC <sub>3</sub> : A Robust Electrode Material for Li, Na, and K Ion Batteries. Journal of Physical Chemistry Letters, 2015, 6, 2728-2732.	2.1	100
18	Density Functional Theory Study of Optical Transitions in Semiconducting Single-Walled Carbon Nanotubes. Nano Letters, 2005, 5, 1621-1624.	4.5	92

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19	Through-Bond and Through-Space $^1J$ Spin-Spin Coupling in Perdifluoronaphthalenes: Accurate DFT Evaluation of the Four Contributions. <i>Journal of the American Chemical Society</i> , 2001, 123, 9162-9163.	6.6	88
20	Screened exchange hybrid density-functional study of the work function of pristine and doped single-walled carbon nanotubes. <i>Journal of Chemical Physics</i> , 2006, 124, 024709.	1.2	87
21	Lithium Adsorption on Graphene: From Isolated Adatoms to Metallic Sheets. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1064-1071.	2.3	79
22	Optical Transitions in Metallic Single-Walled Carbon Nanotubes. <i>Nano Letters</i> , 2005, 5, 1830-1833.	4.5	66
23	Assessment of Density Functionals for Predicting One-Bond Carbon-Hydrogen NMR Spin-Spin Coupling Constants. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 541-545.	2.3	66
24	Natural coupling (NJC) analysis of the electron lone pair effect on NMR couplings: Part 1. The lone pair orientation effect of an $\alpha$ -nitrogen atom on $^1J(\text{C},\text{C})$ couplings. <i>Magnetic Resonance in Chemistry</i> , 2001, 39, 600-606.	1.1	54
25	Theoretical study of the electronic properties of narrow single-walled carbon nanotubes: Beyond the local density approximation. <i>Journal of Chemical Physics</i> , 2004, 121, 10376-10379.	1.2	53
26	Effect of oxygen chemisorption on the energy band gap of a chiral semiconducting single-walled carbon nanotube. <i>Chemical Physics Letters</i> , 2004, 389, 289-292.	1.2	53
27	On the chemical nature of thermally reduced graphene oxide and its electrochemical Li intake capacity. <i>Carbon</i> , 2013, 61, 558-567.	5.4	46
28	Interaction of atomic hydrogen with single-walled carbon nanotubes: A density functional theory study. <i>Journal of Chemical Physics</i> , 2004, 120, 7169-7173.	1.2	44
29	Energy storage capacity of polymeric nitrogen. <i>Molecular Physics</i> , 2006, 104, 745-749.	0.8	42
30	Machine Learning Screening of Metal-Ion Battery Electrode Materials. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 53355-53362.	4.0	42
31	Computational Study of Ortho-Substituent Effects on Antioxidant Activities of Phenolic Dendritic Antioxidants. <i>Antioxidants</i> , 2020, 9, 189.	2.2	41
32	Natural coupling (NJC) analysis of the electron lone pair effect on NMR couplings: 2. The anomeric effects on $^1J(\text{C}, \text{H})$ couplings and its dependence on solvent. <i>Molecular Physics</i> , 2002, 100, 705-715.	0.8	32
33	Tunable Broadband Nanocarbon Transparent Conductor by Electrochemical Intercalation. <i>ACS Nano</i> , 2017, 11, 788-796.	7.3	31
34	Finite perturbation theory-density functional theory calculation of the spin-dipolar contribution to NMR spin-spin coupling constants. <i>Molecular Physics</i> , 2001, 99, 655-661.	0.8	26
35	Density Functional Theory Calculation of Indirect Nuclear Magnetic Resonance Spin-Spin Coupling Constants in C70. <i>Journal of the American Chemical Society</i> , 2004, 126, 7428-7429.	6.6	26
36	Theoretical Nitrogen NMR Chemical Shifts in Octahedral Boron Nitride Cages. <i>Journal of Physical Chemistry A</i> , 2006, 110, 10844-10847.	1.1	26

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37	Vicinal NMR Proton-Proton Coupling Constants. An NBO Analysis. Journal of Physical Chemistry A, 2001, 105, 5298-5303.	1.1	25
38	On the Capriciousness of the FCCF Karplus Curve. Journal of the American Chemical Society, 2002, 124, 9702-9703.	6.6	25
39	Magnetic exchange couplings from noncollinear spin density functional perturbation theory. Journal of Chemical Physics, 2008, 129, 194107.	1.2	24
40	Li adsorption on edge-oxidized graphene nanoribbons predicted by DFT calculations. Surface Science, 2014, 619, 105-113.	0.8	24
41	Solvent Effects on Nuclear Magnetic Resonance $2J(\text{C,Hf})$ and $1J(\text{C,Hf})$ Spin-Spin Coupling Constants in Acetaldehyde. International Journal of Molecular Sciences, 2003, 4, 93-106.	1.8	21
42	$^3J(\text{C1,H3})$ 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
43	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
44	Thickness dependence of solar cell efficiency in transition metal dichalcogenides $\text{MX}_2$ (M: Mo, W; X: S, Se, Te). Journal of Applied Physics, 2013, 114, 093701.	3.0	19
45	Prediction of vicinal proton-proton coupling constants $^3J_{\text{HH}}$ from density functional theory calculations. Molecular Physics, 2005, 103, 1307-1326.	0.8	16
46	Structural and electronic properties of crystalline graphite-like $\text{BC}_3$ . Computational Materials Science, 2015, 109, 248-252.	1.4	11
47	Structure and stability of graphene-like layers built from heterocyclic units. Carbon, 2019, 152, 128-133.	5.4	10
48	Gradient copolymers of thiophene and pyrrole for photovoltaics. Computational Materials Science, 2015, 96, 69-71.	1.4	7
49	The spin-orbit/Fermi contact effect on $^{13}\text{C}$ substituent chemical shifts in 1-halo-bicyclo[1.1.1]pentanes. Molecular Physics, 2003, 101, 1297-1301.	0.8	5
50	Substituent effects on scalar $^1J(^{13}\text{C},^{13}\text{C})$ couplings in pyrimidines. An experimental and DFT study. Magnetic Resonance in Chemistry, 2004, 42, 938-943.	1.1	5
51	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
52	Comparison of oxidized carbon nanotubes for Li-ion storage capacity. Journal of Applied Electrochemistry, 2015, 45, 161-167.	1.5	4
53	Structural and electronic properties of layered nanoporous organic nanocrystals. RSC Advances, 2021, 11, 5773-5784.	1.7	4
54	Theoretical NMR $^1J(^{13}\text{C},^{13}\text{C})$ Scalar Couplings as Probes to Study Diamagnetic Ring Currents in Fullerenes. Advances in Quantum Chemistry, 2005, 127-139.	0.4	3

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55	Synthesis, characterization and DFT study of 1-bromo-4-(3,7-dimethyloctyl)benzene. Journal of Molecular Structure, 2012, 1015, 41-45.	1.8	3
56	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
57	Modeling of Quasi-One-Dimensional Carbon Nanostructures with Density Functional Theory. , 2012, , 901-938.		2
58	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
59	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
60	Gas processing with intrinsically porous 2D membranes. Materials Chemistry and Physics, 2022, 276, 125426.	2.0	2
61	Site-specific polarizabilities from analytic linear-response theory. Chemical Physics Letters, 2014, 608, 24-27.	1.2	0
62	Modeling of Quasi-One-Dimensional Carbon Nanostructures with Density Functional Theory. , 2017, , 1297-1337.		0
63	Modeling of Quasi-One-Dimensional Carbon Nanostructures with Density Functional Theory. , 2015, , 1-41.		0