Carlos Amador-Bedolla

List of Publications by Year
in descending order

51 papers	2,011 citations	471509 17 h-index	243625 44 g-index
59 all docs	59 docs citations	59 times ranked	3149 citing authors

#	Article	IF	Citations
1	Accelerating the discovery of materials for clean energy in the era of smart automation. Nature Reviews Materials, 2018, 3, 5-20.	48.7	489
2	The Harvard Clean Energy Project: Large-Scale Computational Screening and Design of Organic Photovoltaics on the World Community Grid. Journal of Physical Chemistry Letters, 2011, 2, 2241-2251.	4.6	470
3	Accelerated computational discovery of high-performance materials for organic photovoltaics by means of cheminformatics. Energy and Environmental Science, 2011, 4, 4849.	30.8	169
4	Accelerating Resolution-of-the-Identity Second-Order MÃ¸llerâ€“Plesset Quantum Chemistry Calculations with Graphical Processing Units. Journal of Physical Chemistry A, 2008, 112, 2049-2057.	2.5	133
5	Site occupancy of ternary additions to B2 alloys. Intermetallics, 2002, 10, 149-159.	3.9	102
6	Application of generalized gradient-corrected density functionals to iron. Physical Review B, 1992, 46, 1870-1873.	3.2	72
7	Materials Acceleration Platforms: On the way to autonomous experimentation. Current Opinion in Green and Sustainable Chemistry, 2020, 25, 100370.	5.9	67
8	Theoretical and Experimental Study of Relaxations inAl3TiandAl3ZrOrdered Phases. Physical Review Letters, 1995, 74, 4955-4958.	7.8	51
9	Saliva is a reliable and accessible source for the detection of SARS-CoV-2. International Journal of Infectious Diseases, 2021, 105, 83-90.	3.3	47
10	Further insights in DFT calculations of redox potential for iron complexes: The ferrocenium/ferrocene system. Computational and Theoretical Chemistry, 2017, 1099, 167-173.	2.5	35
11	Modelling of the defect structure of Î²-NiAl. Scripta Metallurgica Et Materialia, 1995, 33, 1907-1913.	1.0	33
12	Internal strain effects on the phase diagram of Ni-Pt alloys. Physical Review B, 1993, 47, 15276-15279.	3.2	29
13	An introduction to the BFS method and its use to model binary NiAl alloys. Journal of Computer-Aided Materials Design, 1999, 6, 1-32.	0.7	29
14	Formation energy of disordered alloys from the energetics of ordered compounds. Physical Review B, 1994, 49, 956-960.	3.2	23
15	Band structures of Ni3Pt and NiPt3. Zeitschrift FÃ¼r Physik B-Condensed Matter, 1990, 80, 237-239.	1.1	22
16	"Wrong" Bond Interactions at Inversion Domain Boundaries in GaAs. Physical Review Letters, 1992, 68, 1363-1366.	7.8	22
17	Reassessment of the Four-Point Approach to the Electron-Transfer Marcusâ€“Hush Theory. ACS Omega, 2018, 3, 2130-2140.	3.5	21
18	Electronic structure and nonlinear optical properties of organic photovoltaic systems with potential applications on solar cell devices: a DFT approach. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	17

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19	Zero temperature analysis of the defect structure of B2 FeAl alloys. Scripta Materialia, 1997, 36, 813-819.	5.2	16
20	Factors determining tautomeric equilibria in Schiff bases. Journal of Molecular Structure, 2011, 1006, 600-605.	3.6	14
21	Concentration Effects on the First Reduction Process of Methyl Viologens and Diquat Redox Flow Battery Electrolytes. ACS Applied Energy Materials, 2021, 4, 6624-6634.	5.1	13
22	A comparative DFT study of the catalytic activity of the 3d transition metal sulphides surfaces. Surface Science, 2002, 518, 163-173.	1.9	12
23	Kinetic Properties of Aqueous Organic Redox Flow Battery Anolytes Using the Marcusâ€“Hush Theory. ACS Applied Energy Materials, 2020, 3, 8833-8841.	5.1	12
24	Organic Photovoltaics. , 2013, , 423-442.		10
25	Ruthenium tris bipyridine derivatives and their photocatalytic activity in [4 + 2] cycloadditions. An experimental and DFT study. Catalysis Today, 2018, 310, 2-10.	4.4	10
26	BFS simulation and experimental analysis of the effect of Ti additions on the structure of NiAl. Journal of Computer-Aided Materials Design, 1999, 6, 33-68.	0.7	9
27	Correlating Properties in Iron(III) Complexes: A DFT Description of Structure, Redox Potential and Spin Crossover Phenomena. ChemistrySelect, 2017, 2, 4717-4724.	1.5	9
28	Reagents for electrophilic amination: A quantum Monte Carlo study. Journal of Chemical Physics, 2007, 126, 204308.	3.0	8
29	Theoretical exploration of 2,2â€²-bipyridines as electro-active compounds in flow batteries. Physical Chemistry Chemical Physics, 2019, 21, 15823-15832.	2.8	8
30	Charge-transfer electronic states in organic solar cells: a TDDFT study. Physical Chemistry Chemical Physics, 2021, 23, 16806-16815.	2.8	7
31	Atomistic simulations of bulk heterojunctions to evaluate the structural and packing properties of new predicted donors in OPVs. Physical Chemistry Chemical Physics, 2019, 21, 20315-20326.	2.8	6
32	Promotional effect of Co or Ni impurity in the catalytic activity of MoS2: An electronic structure study. International Journal of Quantum Chemistry, 2000, 80, 406-415.	2.0	5
33	Photoisomerization and its effect in the opto-electronic properties of organic photovoltaic materials: A quantum chemistry study. Journal of Photochemistry and Photobiology A: Chemistry, 2021, 409, 113155.	3.9	5
34	Creating a GUI for Zori, a Quantum Monte Carlo Program. Computing in Science and Engineering, 2009, 11, 41-47.	1.2	4
35	Theoretical analysis of the ?+ Knight shift in Cd and Zn. Hyperfine Interactions, 1981, 8, 483-486.	0.5	3
36	Moment formation in magnetic rare earth metal alloys. Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics, 1985, 130, 37-40.	0.9	3

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37	On the role of driving force in molecular photocells. Physica B: Condensed Matter, 2020, 583, 412052.	2.7	3
38	GPU Algorithm for the Scaled Opposite-Spin (SOS) MP2 Energy Evaluation. Journal of the Mexican Chemical Society, 2017, 61, .	0.6	3
39	Impact of thickness of spin-coated P3HT thin films, over their optical and electronic properties. Journal of Solid State Electrochemistry, 2022, 26, 649-661.	2.5	3
40	Quasiperiodic Branches in the Thermoelectricity of Nanowires. Journal of Electronic Materials, 2019, 48, 5099-5110.	2.2	2
41	Density (de)localization and statistical correlation in the Van der Waals interactions and the chemical bond between two hydrogens. Physica A: Statistical Mechanics and Its Applications, 2019, 527, 121324.	2.6	2
42	Experimental and Theoretical Exploration of Aryl Substituent Effects on the Electronic Properties of Asymmetric 4,7-Di(thiophene-2-yl)-benzo[c][2,1,5]thiadiazole Compounds. Polycyclic Aromatic Compounds, 2020, , 1-16.	2.6	2
43	Isomerization reactions with [Ru(Bpy)3]2+ photocatalyst. A DFT study of the factors influencing the energy transfer mechanism supported by experimental data. Journal of Photochemistry and Photobiology A: Chemistry, 2021, 414, 113224.	3.9	2
44	Chemical bonding and structural relaxation of amorphous ZrxCu1â^'x. Journal of Non-Crystalline Solids, 1985, 75, 385-390.	3.1	1
45	A Synergetic Experimental and Computational Approach Towards a Better Comprehension of Redox		