David Santos-Carballal

List of Publications by Year
in descending order

42	968	471509 17	454955 30
papers	citations	h-index	g-index

42	42	42	1128
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A DFT study of the structures, stabilities and redox behaviour of the major surfaces of magnetite Fe₃O₄. Physical Chemistry Chemical Physics, 2014, 16, 21082-21097.	2.8	178
2	First-principles study of the inversion thermodynamics and electronic structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Fe</mml:mi><mml:msub><mml:mi>M</mml:mi><mml:mi><mml:m		

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19	Ethylene carbonate adsorption on the major surfaces of lithium manganese oxide Li_{1â^'x}Mn₂O₄spinel (0.000 <i>x< 0.375): a DFT+U-D3 study. Physical Chemistry Chemical Physics, 2020, 22, 6763-6771.	2.8	18
20	CO₂ interaction with violarite (FeNi₂S₄) surfaces: a dispersion-corrected DFT study. Physical Chemistry Chemical Physics, 2018, 20, 20439-20446.	2.8	15
21	Al₂O₃/ZnO Heterostructure-Based Sensors for Volatile Organic Compounds in Safety Applications. ACS Applied Materials & Interfaces, 2022, 14, 29331-29344.	8.0	15
22	Atomistic Molecular Dynamics Simulations of Propofol and Fentanyl in Phosphatidylcholine Lipid Bilayers. ACS Omega, 2020, 5, 14340-14353.	3.5	14
23	Synthesis, Crystal Structures, and Properties of Zeoliteâ€Like T₃(H₃O)₂[M(CN)₆]₂Â·uH₂O (T = Co, Zn; M = Ru, Os). European Journal of Inorganic Chemistry, 2017, 2017, 2980-2989.	2.0	13
24	CO₂ reduction to acetic acid on the greigite Fe₃S₄{111} surface. Faraday Discussions, 2021, 229, 35-49.	3.2	12
25	Catalytic Conversion of CO and H₂ into Hydrocarbons on the Cobalt Co(111) Surface: Implications for the Fischerâ€“Tropsch Process. Journal of Physical Chemistry C, 2021, 125, 11891-11903.	3.1	11
26	Density Functional Theory Study of Ethylene Carbonate Adsorption on the (0001) Surface of Aluminum Oxide Î±-Al₂O₃. ACS Omega, 2021, 6, 29577-29587.	3.5	11
27	Mixing thermodynamics and electronic structure of the Pt_{1â^'x}Ni_x (0 â‰¤ Tj ETQq1 1 0.784314 rgBT /Over	3.6	10
28	Interaction of SO2 with the Platinum (001), (011), and (111) Surfaces: A DFT Study. Catalysts, 2020, 10, 558.	3.5	9
29	Density Functional Theory Study of Monoclinic FeNbO₄: Bulk Properties and Water Dissociation at the (010), (011), (110), and (111) Surfaces. Journal of Physical Chemistry C, 2021, 125, 27566-27577.	3.1	6
30	A computational study of the interaction of organic surfactants with goethite Î±-FeO(OH) surfaces. RSC Advances, 2016, 6, 91893-91903.	3.6	5
31	DFT analysis of rotational barriers, 1H and 13C NMR chemical shifts in neutral and protonated furfurylidenanilines. Computational and Theoretical Chemistry, 2008, 852, 78-82.	1.5	3
32	Thermal Properties and Segregation Behavior of Pt Nanowires Modified with Au, Ag, and Pd Atoms: A Classical Molecular Dynamics Study. Journal of Physical Chemistry C, 2019, 123, 20522-20531.	3.1	2
33	Competitive Adsorption of H2O and SO2 on Catalytic Platinum Surfaces: a Density Functional Theory Study. South African Journal of Chemistry, 2021, 74, .	0.6	2
34	DFT+U Study of the Electronic, Magnetic and Mechanical Properties of Co, CoO, and Co3O4. South African Journal of Chemistry, 2021, 74, .	0.6	2
35	Controlling the Lithium Intercalation Voltage in the Li(Mn1-xNix)2O4 Spinel via Tuning of the Ni Concentration: a Density Functional Theory Study. South African Journal of Chemistry, 2021, 74, .	0.6	2
36	Conformational and NMR study of some furan derivatives by DFT methods. Journal of Molecular Modeling, 2013, 19, 4591-4601.	1.8	1

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37	Thermodynamics of the Atomic Distribution in Pt3Pd2, Pt2Pd3 and their Corresponding (111) Surfaces. South African Journal of Chemistry, 2021, 74, .	0.6	1
38	Density Functional Theory Study of the Adsorption of Oxygen and Hydrogen on 3d Transition Metal Surfaces with Varying Magnetic Ordering. South African Journal of Chemistry, 2021, 74, .	0.6	1
39	Theory: general discussion. Faraday Discussions, 2021, 229, 131-160.	3.2	0
40	A Dft+U Study of the Oxidation of Cobalt Nanoparticles: Implications for Biomedical Applications. SSRN Electronic Journal, 0, , .	0.4	0
41	Controlling the Lithium Intercalation Voltage in the Li(Mn1-x Ni x)2O4 Spinel Via Tuning of the Ni Concentration: A Density Functional Theory Study.. ECS Meeting Abstracts, 2020, MA2020-02, 3815-3815.	0.0	0
42	Africa-UK Partnership for the Computer-aided Development of Sustainable Catalysts. South African Journal of Chemistry, 2021, 74, .	0.6	0