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	Al₂O₃/ZnO Heterostructure-Based Sensors for Volatile Organic Compounds in Safety Applications. ACS Applied Materials & Interfaces, 2022, 14, 29331-29344.	8.0	15
2	CO₂ reduction to acetic acid on the greigite Fe₃S₄{111} surface. Faraday Discussions, 2021, 229, 35-49.	3.2	12
3	Theory: general discussion. Faraday Discussions, 2021, 229, 131-160.	3.2	0
4	The role of surface oxidation and Feâ€“Ni synergy in Feâ€“Niâ€“S catalysts for CO₂ hydrogenation. Faraday Discussions, 2021, 230, 30-51.	3.2	21
5	Competitive adsorption geometries for the arsenate As(V) and phosphate P(V) oxyanions on magnetite surfaces: Experiments and theory. American Mineralogist, 2021, 106, 374-388.	1.9	24
6	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
7	TiO₂/Cu₂O/CuO Multi-Nanolayers as Sensors for H₂ and Volatile Organic Compounds: An Experimental and Theoretical Investigation. ACS Applied Materials & Interfaces, 2021, 13, 32363-32380.	8.0	39
8	Tailoring the selectivity of ultralow-power heterojunction gas sensors by noble metal nanoparticle functionalization. Nano Energy, 2021, 88, 106241.	16.0	21
9	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
10	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
11	A NIR-II-emitting gold nanocluster-based drug delivery system for smartphone-triggered photodynamic theranostics with rapid body clearance. Materials Today, 2021, 51, 96-107.	14.2	26
12	Thermodynamics of the Atomic Distribution in Pt3Pd2, Pt2Pd3 and their Corresponding (111) Surfaces. South African Journal of Chemistry, 2021, 74, .	0.6	1
13	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
14	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
15	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
16	Africa-UK Partnership for the Computer-aided Development of Sustainable Catalysts. South African Journal of Chemistry, 2021, 74, .	0.6	0
17	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
18	Surface functionalization of ZnO:Ag columnar thin films with AgAu and AgPt bimetallic alloy nanoparticles as an efficient pathway for highly sensitive gas discrimination and early hazard detection in batteries. Journal of Materials Chemistry A, 2020, 8, 16246-16264.	10.3	38

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19	Atomistic Molecular Dynamics Simulations of Propofol and Fentanyl in Phosphatidylcholine Lipid Bilayers. ACS Omega, 2020, 5, 14340-14353.	3.5	14
20	Interaction of SO2 with the Platinum (001), (011), and (111) Surfaces: A DFT Study. Catalysts, 2020, 10, 558.	3.5	9
21	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
22	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
23	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
24	Tuning ZnO Sensors Reactivity toward Volatile Organic Compounds via Ag Doping and Nanoparticle Functionalization. ACS Applied Materials & Interfaces, 2019, 11, 31452-31466.	8.0	78
25	Interaction of H₂O with the Platinum Pt (001), (011), and (111) Surfaces: A Density Functional Theory Study with Long-Range Dispersion Corrections. Journal of Physical Chemistry C, 2019, 123, 27465-27476.	3.1	33
26	A DFT+U study of the oxidation of cobalt nanoparticles: Implications for biomedical applications. Materialia, 2019, 7, 100381.	2.7	25
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	Ab initio investigation of the thermodynamics of cation distribution and of the electronic and magnetic structures in the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>LiMn</mml:mi><mml:mn>2</mml:mn><mml:mn></mn mathvariant="normal">O</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math> spinel. Physical Review B, 2018, 97, .	3.2	21
29	Reactivity of CO ₂ on the surfaces of magnetite (Fe ₃ O ₄), greigite (Fe ₃ S ₄) and mackinawite (FeS). Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2018, 376, 20170065.	3.4	27
30	Tuning doping and surface functionalization of columnar oxide films for volatile organic compound sensing: experiments and theory. Journal of Materials Chemistry A, 2018, 6, 23669-23682.	10.3	36
31	CO₂ interaction with violarite (FeNi₂S₄) surfaces: a dispersion-corrected DFT study. Physical Chemistry Chemical Physics, 2018, 20, 20439-20446.	2.8	15
32	Insight into the Nature of Iron Sulfide Surfaces During the Electrochemical Hydrogen Evolution and CO₂ Reduction Reactions. ACS Applied Materials & Interfaces, 2018, 10, 32078-32085.	8.0	33
33	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
34	Early Oxidation Processes on the Greigite Fe₃S₄(001) Surface by Water: A Density Functional Theory Study. Journal of Physical Chemistry C, 2016, 120, 8616-8629.	3.1	32
35	A computational study of the interaction of organic surfactants with goethite Î±-FeO(OH) surfaces. RSC Advances, 2016, 6, 91893-91903.	3.6	5
36	A density functional theory study of uranium-doped thoria and uranium adatoms on the major surfaces of thorium dioxide. Journal of Nuclear Materials, 2016, 473, 99-111.	2.7	28

#	Article	IF	Citations
37	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>		