Juarez L F Da Silva

List of Publications by Citations

166 papers	6,465 citations	40 h-index	76 g-index
180 ext. papers	7,218 ext. citations	4 avg, IF	6.22 L-index

#	Paper	IF	Citations
166	Nature of the band gap of In2O3 revealed by first-principles calculations and x-ray spectroscopy. *Physical Review Letters*, **2008**, 100, 167402	7.4	498
165	Hybrid functionals applied to rare-earth oxides: The example of ceria. *Physical Review B*, **2007**, 75,	3.3	461
164	Density-functional calculations of the structure of near-surface oxygen vacancies and electron localization on CeO2(111). *Physical Review Letters*, **2009**, 102, 026101	7.4	442
163	Theoretical description of carrier mediated magnetism in cobalt doped ZnO. *Physical Review Letters* , **2008**, 100, 256401	7.4	240
162	Origins of band-gap renormalization in degenerately doped semiconductors. *Physical Review B*, **2008**, 78,	3.3	235
161	Converged properties of clean metal surfaces by all-electron first-principles calculations. *Surface Science*, **2006**, 600, 703-715	1.8	225
160	Density functional theory investigation of 3d, 4d, and 5d 13-atom metal clusters. *Physical Review B*, **2010**, 81,	3.3	180
159	Revised ab initio natural band offsets of all group IV, II-VI, and III-V semiconductors. *Applied Physics Letters*, **2009**, 94, 212109	3.4	162
158	Spin-orbit coupling and ion displacements in multiferroic TbMnO3. *Physical Review Letters*, **2008**, 101, 037209	7.4	158
157	Adsorption of Xe atoms on metal surfaces: new insights from first-principles calculations. *Physical Review Letters*, **2003**, 90, 066104	7.4	158
156	Insights into the structure of the stable and metastable (GeTe)m(Sb2Te3)n compounds. *Physical Review B*, **2008**, 78,	3.3	147
155	Cohesive properties of group-III nitrides: A comparative study of all-electron and pseudopotential calculations using the generalized gradient approximation. *Physical Review B*, **2002**, 65,	3.3	118
154	Optical properties of pseudobinary GeTe, Ge2Sb2Te5, GeSb2Te4, GeSb4Te7, and Sb2Te3 from ellipsometry and density functional theory. *Physical Review B*, **2009**, 80,	3.3	110
153	Effect of copassivation of Cl and Cu on CdTe grain boundaries. *Physical Review Letters*, **2008**, 101, 155501	7.4	95
152	Electronic structure of In2O3 and Sn-doped In2O3 by hard x-ray photoemission spectroscopy. *Physical Review B*, **2010**, 81,	3.3	94
151	Xe adsorption on metal surfaces: First-principles investigations. *Physical Review B*, **2005**, 72,	3.3	90
150	Ethanol and Water Adsorption on Close-Packed 3d, 4d, and 5d Transition-Metal Surfaces: A Density Functional Theory Investigation with van der Waals Correction. *Journal of Physical Chemistry C*, **2012**, 116, 24695-24705	3.8	87

149	Comment on "Taming multiple valency with density functionals: A case study of defective ceria" *Physical Review B*, **2005**, 72,	3.3	81
148	Interplay between Order and Disorder in the High Performance of Amorphous Transparent Conducting Oxides. *Chemistry of Materials*, **2009**, 21, 5119-5124	9.6	80
147	Revised basin-hopping Monte Carlo algorithm for structure optimization of clusters and nanoparticles. *Journal of Chemical Information and Modeling*, **2013**, 53, 2282-98	6.1	79
146	The role of charge states in the atomic structure of Cu(n) and Pt(n) (n = 2-14 atoms) clusters: a DFT investigation. *Journal of Physical Chemistry A*, **2014**, 118, 10813-21	2.8	77
145	Evolution of the structural, energetic, and electronic properties of the 3d, 4d, and 5d transition-metal clusters (30 TM systems for n = 2-15): a density functional theory investigation. *Physical Chemistry Chemical Physics*, **2017**, 19, 15484-15502	3.6	74
144	Origin of electronic and optical trends in ternary In2O3(ZnO)n transparent conducting oxides (n=1,3,5): Hybrid density functional theory calculations. *Physical Review B*, **2009**, 79,	3.3	73
143	Effective coordination concept applied for phase change (GeTe)m(Sb2Te3)n compounds. *Journal of Applied Physics*, **2011**, 109, 023502	2.5	72
142	Stability of the Ce2O3 phases: A DFT+U investigation. *Physical Review B*, **2007**, 76,	3.3	70
141	Strain relaxation and band-gap tunability in ternary InxGa1−xN nanowires. *Physical Review B*, **2008**, 78,	3.3	67
140	Rules of structure formation for the homologous InMO3(ZnO)n compounds. *Physical Review Letters*, **2008**, 100, 255501	7.4	59
139	Theoretical Study of the Structural, Energetic, and Electronic Properties of 55-Atom Metal Nanoclusters: A DFT Investigation within van der Waals Corrections, Spin−Orbit Coupling, and PBE+U of 42 Metal Systems. *Journal of Physical Chemistry C*, **2016**, 120, 28844-28856	3.8	59
138	Formation of the cerium orthovanadate CeVO4: DFT+U study. *Physical Review B*, **2007**, 76,	3.3	56
137	Stability and electronic structures of CuxTe. *Applied Physics Letters*, **2007**, 91, 091902	3.4	54
136	Platinum-Based Nanoalloys PtnTM55−n (TM = Co, Rh, Au): A Density Functional Theory Investigation. *Journal of Physical Chemistry C*, **2012**, 116, 18432-18439	3.8	53
135	Structure, Electronic, and Magnetic Properties of Binary PtnTM55−n (TM = Fe, Co, Ni, Cu, Zn) Nanoclusters: A Density Functional Theory Investigation. *Journal of Physical Chemistry C*, **2015**, 119, 15669-15679	3.8	51
134	All-electron first-principles calculations of clean surface properties of low-Miller-index Al surfaces. *Physical Review B*, **2005**, 71,	3.3	51
133	Reconstruction of core and surface nanoparticles: The example of Pt55 and Au55. *Physical Review B*, **2010**, 82,	3.3	50
132	Trends in adsorption of noble gases He, Ne, Ar, Kr, and Xe on Pd(111)(3×3)R30°: All-electron density-functional calculations. *Physical Review B*, **2008**, 77,	3.3	50

131	Theory of nitride oxide adsorption on transition metal (111) surfaces: a first-principles investigation. *Physical Chemistry Chemical Physics*, **2010**, 12, 2459-70	3.6	49
130	All-electron first-principles investigations of the energetics of vicinal Cu surfaces. *Physical Review B*, **2006**, 73,	3.3	48
129	Establishing a Link between Well-Ordered Pt(100) Surfaces and Real Systems: How Do Random Superficial Defects Influence the Electro-oxidation of Glycerol?. *ACS Catalysis*, **2015**, 5, 4227-4236	13.1	44
128	Optical properties of (GeTe, Sb2Te3) pseudobinary thin films studied with spectroscopic ellipsometry. *Applied Physics Letters*, **2008**, 93, 021914	3.4	44
127	Density functional theory study of the energetics, electronic structure, and core-level shifts of NO adsorption on the Pt(111) surface. *Physical Review B*, **2009**, 79,	3.3	43
126	Multi-component transparent conducting oxides: progress in materials modelling. *Journal of Physics Condensed Matter*, **2011**, 23, 334210	1.8	39
125	Quantum Monte Carlo study of small aluminum clusters Aln (n=2–13). *Physical Review B*, **2012**, 85,	3.3	39
124	The role of electron localization in the atomic structure of transition-metal 13-atom clusters: the example of Co13, Rh13, and Hf13. *Physical Chemistry Chemical Physics*, **2011**, 13, 17242-8	3.6	38
123	Graphene-supported small transition-metal clusters: A density functional theory investigation within van der Waals corrections. *Physical Review B*, **2017**, 95,	3.3	36
122	The role of charge transfer in the oxidation state change of Ce atoms in the TM13-CeO2(111) systems (TM = Pd, Ag, Pt, Au): a DFT + U investigation. *Physical Chemistry Chemical Physics*, **2015**, 17, 13520-30	3.6	35
121	Structural formation of binary PtCu clusters: A density functional theory investigation. *Computational Materials Science*, **2015**, 98, 278-286	3.2	34
120	Adsorption of Rh, Pd, Ir, and Pt on the Au(111) and Cu(111) Surfaces: A Density Functional Theory Investigation. *Journal of Physical Chemistry C*, **2014**, 118, 19051-19061	3.8	34
119	First-principles investigation of the multilayer relaxation of stepped Cu surfaces. *Physical Review B*, **2004**, 69,	3.3	34
118	Comparative study of van der Waals corrections to the bulk properties of graphite. *Journal of Physics Condensed Matter*, **2015**, 27, 415502	1.8	32
117	Hybrid density functional study of small Rhn (n=2–15) clusters. *Physical Review B*, **2012**, 86,	3.3	32
116	Ethanol and Water Adsorption on Transition-Metal 13-Atom Clusters: A Density Functional Theory Investigation within van der Waals Corrections. *Journal of Physical Chemistry A*, **2016**, 120, 4231-40	2.8	31
115	Glycerol Adsorption on Platinum Surfaces: A Density Functional Theory Investigation with van der Waals Corrections. *Journal of Physical Chemistry C*, **2014**, 118, 15251-15259	3.8	31
114	How do random superficial defects influence the electro-oxidation of glycerol on Pt(111) surfaces?. *Physical Chemistry Chemical Physics*, **2016**, 18, 25582-25591	3.6	30

113	Atomic structure of In2O3(ZnO) systems. *Applied Physics Letters*, **2007**, 90, 261904	3.4	30
112	Theoretical Investigation of Small Transition-Metal Clusters Supported on the CeO2(111) Surface. *Journal of Physical Chemistry C*, **2014**, 118, 21438-21446	3.8	29
111	Adsorption of NO on the Rh13, Pd13, Ir13, and Pt13 Clusters: A Density Functional Theory Investigation. *Journal of Physical Chemistry C*, **2012**, 116, 20540-20549	3.8	29
110	Encapsulation of small magnetic clusters in fullerene cages: A density functional theory investigation within van der Waals corrections. *Physical Review B*, **2012**, 85,	3.3	29
109	Bulk structures of PtO and PtO2 from density functional calculations. *Physical Review B*, **2011**, 84,	3.3	29
108	Atomistic origins of the phase transition mechanism in Ge2Sb2Te5. *Journal of Applied Physics*, **2009**, 106, 113509	2.5	28
107	Theoretical investigation of atomic and electronic structures of Ga2O3(ZnO)6. *Physical Review B*, **2009**, 80,	3.3	26
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105	The Mackay-Type Cluster [Cu Al](Cp*) : Open-Shell 67-Electron Superatom with Emerging Metal-Like Electronic Structure. *Angewandte Chemie - International Edition*, **2018**, 57, 14630-14634	16.4	25
104	Density Functional Investigation of the Adsorption of Ethanol–Water Mixture on the Pt(111) Surface. *Journal of Physical Chemistry C*, **2013**, 117, 16942-16952	3.8	25
103	Nature of Xenon adsorption on graphite: On-top versus hollow site preference. *Physical Review B*, **2007**, 76,	3.3	25
102	Adsorption of water and ethanol on noble and transition-metal substrates: a density functional investigation within van der Waals corrections. *Physical Chemistry Chemical Physics*, **2016**, 18, 29526-29536	3.6	25
101	Theoretical Investigation of the Adsorption Properties of CO, NO, and OH on Monometallic and Bimetallic 13-Atom Clusters: The Example of Cu13, Pt7Cu6, and Pt13. *Journal of Physical Chemistry A*, **2015**, 119, 11565-73	2.8	24
100	Transition-metal 13-atom clusters assessed with solid and surface-biased functionals. *Journal of Chemical Physics*, **2011**, 134, 134105	3.9	24
99	Ferrimagnetic Fe-doped GaN: An unusual magnetic phase in dilute magnetic semiconductors. *Physical Review B*, **2009**, 79,	3.3	24
98	Ab initio investigation of structural stability and exfoliation energies in transition metal dichalcogenides based on Ti-, V-, and Mo-group elements. *Physical Review Materials*, **2019**, 3,	3.2	24
97	Role of van der Waals corrections for the PtX2 (X=O, S, Se) compounds. *Physical Review B*, **2013**, 88,	3.3	23
96	Understanding the clean interface between covalent Si and ionic Al2O3. *Physical Review Letters*, **2009**, 103, 116101	7.4	20

95	Ab initio investigation of the atomistic descriptors in the activation of small molecules on 3d transition-metal 13-atom clusters: The example of H, CO, HO, and CO. *Journal of Chemical Physics*, **2019**, 151, 214301	3.9	19
94	Physical and Chemical Properties of Unsupported (MO2)n Clusters for M = Ti, Zr, or Ce and n = 1□5: A Density Functional Theory Study Combined with the Tree-Growth Scheme and Euclidean Similarity Distance Algorithm. *Journal of Physical Chemistry C*, **2018**, 122, 27702-27712	3.8	19
93	The role of the CO adsorption on Pt monolayers supported on flat and stepped Au surfaces: a density functional investigation. *RSC Advances*, **2014**, 4, 9247-9254	3.7	18
92	Correlation between the electronic structures and diffusion paths of interstitial defects in semiconductors: The case of CdTe. *Physical Review B*, **2014**, 90,	3.3	18
91	Role of atomic radius and d-states hybridization in the stability of the crystal structure of M2O3 (M=Al, Ga, In) oxides. *Physical Review B*, **2014**, 90,	3.3	18
90	Trend for the multilayer relaxation sequence of stepped Cu surfaces. *Physical Review B*, **2004**, 70,	3.3	18
89	Ab Initio Investigation of Atomistic Insights into the Nanoflake Formation of Transition-Metal Dichalcogenides: The Examples of MoS2, MoSe2, and MoTe2. *Journal of Physical Chemistry C*, **2018**, 122, 27059-27069	3.8	18
88	Density functional theory and ab initio molecular dynamics study of NO adsorption on Pd(111) and Pt(111) surfaces. *Physical Review B*, **2010**, 81,	3.3	15
87	Machine Learning Prediction of Nine Molecular Properties Based on the SMILES Representation of the QM9 Quantum-Chemistry Dataset. *Journal of Physical Chemistry A*, **2020**, 124, 9854-9866	2.8	15
86	The Role of Low-Coordinated Sites on the Adsorption of Glycerol on Defected Ptn/Pt(111) Substrates: A Density Functional Investigation within the D3 van der Waals Correction. *Journal of Physical Chemistry C*, **2017**, 121, 3445-3454	3.8	13
85	Ab initio investigation of quantum size effects on the adsorption of CO, CO, HO, and H on transition-metal particles. *Physical Chemistry Chemical Physics*, **2020**, 22, 8998-9008	3.6	13
84	A comprehensive study of g-factors, elastic, structural and electronic properties of III-V semiconductors using hybrid-density functional theory. *Journal of Applied Physics*, **2018**, 123, 065702	2.5	13
83	Origin of and tuning the optical and fundamental band gaps in transparent conducting oxides: The case of M2O3(M=Al,Ga,In). *Physical Review B*, **2015**, 92,	3.3	13
82	Structural and electronic properties of TM23 - pAgp (TM = Ni, Pd, and Pt) clusters in the dilute limit (p = 0□): A density functional theory investigation. *European Physical Journal D*, **2013**, 67, 1	1.3	13
81	Publisher's Note: Hybrid functionals applied to rare-earth oxides: The example of ceria [Phys. Rev. B 75, 045121 (2007)]. *Physical Review B*, **2007**, 75,	3.3	13
80	The influence of hydroxy groups on the adsorption of three-carbon alcohols on Ni(111), Pd(111) and Pt(111) surfaces: a density functional theory study within the D3 dispersion correction. *Physical Chemistry Chemical Physics*, **2019**, 21, 8434-8444	3.6	12
79	Ab Initio Investigation of the Role of Atomic Radius in the Structural Formation of PtnTM55□ (TM = Y, Zr, Nb, Mo, and Tc) Nanoclusters. *Journal of Physical Chemistry C*, **2018**, 122, 7444-7454	3.8	12
78	First-Principles Exploration of Two-Dimensional Transition Metal Dichalcogenides Based on Fe, Co, Ni, and Cu Groups and Their van der Waals Heterostructures. *ACS Applied Energy Materials*, **2019**, 2, 8491-8501	6.1	12

77	Adsorption of CO, NO, and H2 on the PdnAu55−n Nanoclusters: A Density Functional Theory Investigation within the van der Waals D3 Corrections. *Journal of Physical Chemistry C*, **2019**, 123, 7431-7439	3.8	11
76	Size-Induced Phase Evolution of MoSe2 Nanoflakes Revealed by Density Functional Theory. *Journal of Physical Chemistry C*, **2018**, 122, 20483-20488	3.8	11
75	The adsorption of alcohols on strained PtNi(111) substrates: a density functional investigation within the D3 van der Waals correction. *Physical Chemistry Chemical Physics*, **2018**, 20, 24210-24221	3.6	11
74	Investigation of CO Adsorption on 13-Atom 4d Clusters. *Journal of Chemical Information and Modeling*, **2020**, 60, 537-545	6.1	11
73	Ab Initio Insights into the Formation Mechanisms of 55-Atom Pt-Based Core−Shell Nanoalloys. *Journal of Physical Chemistry C*, **2020**, 124, 1158-1164	3.8	11
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71	Water adsorption on the stoichiometric and defected Fe(110) surfaces. *Surface Science*, **2018**, 668, 144-149	1.9	11
70	First-principles investigation of the role of registry relaxations on stepped Cu(100) surfaces. *Physical Review B*, **2005**, 72,	3.3	10
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68	Tuning the Magnetic Properties of FeCo Thin Films through the Magnetoelastic Effect Induced by the Au Underlayer Thickness. *ACS Applied Materials & Interfaces*, **2019**, 11, 1529-1537	9.5	10
67	Optical and fundamental band gaps disparity in transparent conducting oxides: new findings for the [Formula: see text] and [Formula: see text] systems. *Journal of Physics Condensed Matter*, **2017**, 29, 085501	1.8	9
66	Electronic structure of layered quaternary chalcogenide materials for band-gap engineering: The example of Cs2MIIM3IVQ8. *Physical Review B*, **2016**, 93,	3.3	9
65	Azobenzene Adsorption on the MoS2(0001) Surface: A Density Functional Investigation within van der Waals Corrections. *Journal of Physical Chemistry C*, **2018**, 122, 18895-18901	3.8	9
64	Ab Initio Investigation of the Role of CO Adsorption on the Physical Properties of 55-Atom PtCo Nanoalloys. *Journal of Physical Chemistry C*, **2017**, 121, 27721-27732	3.8	9
63	Electronic Structure and Stability of Be Impurities in Cubic Boron Nitride. *Physica Status Solidi (B): Basic Research*, **1998**, 210, 401-405	1.3	9
62	A theoretical investigation of the structural and electronic properties of 55-atom nanoclusters: The examples of Y-Tc and Pt. *Journal of Chemical Physics*, **2016**, 144, 054310	3.9	9
61	The role of the cationic Pt sites in the adsorption properties of water and ethanol on the Pt/Pt(111) and Pt/CeO(111) substrates: A density functional theory investigation. *Journal of Chemical Physics*, **2016**, 145, 124709	3.9	9
60	Stability and accuracy control of k·p parameters. *Semiconductor Science and Technology*, **2016**, 31, 105002	2.3	8

59	Carrier-induced enhancement and suppression of ferromagnetism in Zn1-xCrxTe and Ga1-xCrxAs: origin of the spinodal decomposition. *New Journal of Physics*, **2008**, 10, 113007	2.9	8
58	Theoretical Investigation of the Na+ Transport Mechanism and the Performance of Ionic Liquid-Based Electrolytes in Sodium-Ion Batteries. *ACS Applied Energy Materials*, **2021**, 4, 4444-4458	6.1	8
57	Thermodynamic properties of 55-atom Pt-based nanoalloys: Phase changes and structural effects on the electronic properties. *Journal of Chemical Physics*, **2019**, 151, 204301	3.9	8
56	Density functional investigation of the adsorption effects of PH and SH on the structure stability of the Au and Pt nanoclusters. *Journal of Chemical Physics*, **2017**, 146, 164304	3.9	7
55	Parallel tempering Monte Carlo combined with clustering Euclidean metric analysis to study the thermodynamic stability of Lennard-Jones nanoclusters. *Journal of Chemical Physics*, **2017**, 146, 064114	3.9	7
54	Atomic structure of the La/Pt(111) and Ce/Pt(111) surfaces revealed by DFT+U calculations. *RSC Advances*, **2015**, 5, 521-528	3.7	7
53	Walsh, Da Silva, and Wei Reply:. *Physical Review Letters*, **2009**, 102,	7.4	7
52	Interfacial Structures in Ionic Liquid-Based Ternary Electrolytes for Lithium-Metal Batteries: A Molecular Dynamics Study. *Journal of Physical Chemistry B*, **2020**, 124, 9648-9657	3.4	7
51	Novel zero-dimensional lead-free bismuth based perovskites: from synthesis to structural and optoelectronic characterization. *Materials Advances*, **2020**, 1, 3439-3448	3.3	7
50	Unveiling the adsorption properties of 3d, 4d, and 5d metal adatoms on the MoS2 monolayer: A DFT-D3 investigation. *Surface Science*, **2020**, 701, 121700	1.8	7
49	Methane dehydrogenation on 3d 13-atom transition-metal clusters: A density functional theory investigation combined with Spearman rank correlation analysis. *Fuel*, **2020**, 275, 117790	7.1	6
48	Nitroxyl as a ligand in ruthenium tetraammine systems: a density functional theory study. *Dalton Transactions*, **2016**, 45, 4907-15	4.3	6
47	Evidence for a subtle structural symmetry breaking in EuB(6). *Journal of Physics Condensed Matter*, **2009**, 21, 456007	1.8	6
46	Linear scaling of the interlayer relaxations of the vicinal Cu(p,p,p□) surfaces with the number of atom-rows in the terraces. *Surface Science*, **2006**, 600, 3008-3014	1.8	6
45	Role of Structural Phases and Octahedra Distortions in the Optoelectronic and Excitonic Properties of CsGeX3 (X = Cl, Br, I) Perovskites. *Journal of Physical Chemistry C*, **2021**, 125, 19142-19155	3.8	6
44	The role of the alkali and chalcogen atoms on the stability of the layered chalcogenide [Formula: see text] (A = alkali-metal; M = metal-cations; Q = chalcogen) compounds: a density functional theory investigation within van der Waals corrections. *Journal of Physics Condensed Matter*, **2017**,	1.8	5
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42	Interplay between structure asymmetry, defect-induced localization, and spin-orbit interaction in Mn-doped quantum dots. *Physical Review B*, **2017**, 95,	3.3	5

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40	Optical and dielectric properties of lead perovskite and iodoplumbate complexes: an ab initio study. *Physical Chemistry Chemical Physics*, **2020**, 22, 18423-18434	3.6	5
39	Beyond the Anderson rule: importance of interfacial dipole and hybridization in van der Waals heterostructures. *2D Materials*, **2021**, 8, 041002	5.9	5
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37	(Meta-)stability and Core-Shell Dynamics of Gold Nanoclusters at Finite Temperature. *Journal of Physical Chemistry Letters*, **2019**, 10, 685-692	6.4	4
36	Contrasting Structure and Bonding of a Copper-Rich and a Zinc-Rich Intermetalloid Cu/Zn Cluster. *Inorganic Chemistry*, **2020**, 59, 9077-9085	5.1	4
35	The role of the A-cations in the polymorphic stability and optoelectronic properties of lead-free ASnI perovskites. *Physical Chemistry Chemical Physics*, **2021**, 23, 2286-2297	3.6	4
34	investigation of the formation of ZrO-like structures upon the adsorption of Zr on the CeO(111) surface. *Journal of Chemical Physics*, **2018**, 149, 244702	3.9	4
33	Polyhydroxamicalkanoate as a bioinspired acetylcholinesterase-based catalyst for acetylthiocholine hydrolysis and organophosphorus dephosphorylation: experimental studies and theoretical insights. *Catalysis Science and Technology*, **2017**, 7, 3388-3398	5.5	3
32	Mixed Halide Lead-free Double Perovskite Alloys for Band Gap Engineering. *ACS Applied Energy Materials*, **2020**, 3, 7364-7371	6.1	3
31	Ab initio investigation of the role of transition-metal dopants in the adsorption properties of ethylene glycol on doped Pt(100) surfaces. *Physical Chemistry Chemical Physics*, **2020**, 22, 17646-17658	3.6	3
30	Investigation of the Stability Mechanisms of Eight-Atom Binary Metal Clusters Using DFT Calculations and -means Clustering Algorithm. *Journal of Chemical Information and Modeling*, **2021**, 61, 3411-3420	6.1	3
29	Systematic Investigation of Error Distribution in Machine Learning Algorithms Applied to the Quantum-Chemistry QM9 Data Set Using the Bias and Variance Decomposition. *Journal of Chemical Information and Modeling*, **2021**, 61, 4210-4223	6.1	3
28	screening of Pt-based transition-metal nanoalloys using descriptors derived from the adsorption and activation of CO. *Physical Chemistry Chemical Physics*, **2021**, 23, 6029-6041	3.6	3
27	Ab initio investigation of the role of the d-states occupation on the adsorption properties of H, CO, CH and CHOH on the Fe, Co, Ni and Cu clusters. *Physical Chemistry Chemical Physics*, **2021**, 23, 8739-8751	3.6	3
26	The role of site coordination on the CO2 electroreduction pathway on stepped and defective copper surfaces. *Catalysis Science and Technology*, **2021**, 11, 2770-2781	5.5	3
25	On a high photocatalytic activity of high-noble alloys Au-Ag/TiO catalysts during oxygen evolution reaction of water oxidation.. *Scientific Reports*, **2022**, 12, 2604	4.9	3
24	Defect-induced magnetism in II-VI quantum dots. *Physical Review B*, **2019**, 99,	3.3	2

23	Exploring the adsorption site coordination as a strategy to tune copper catalysts for CO2 electro-reduction. *Catalysis Science and Technology*, **2022**, 12, 869-879	5.5	2
22	Ab Initio Study of the C□O Bond Dissociation in CO2 Reduction by Redox and Carboxyl Routes on 3d Transition Metal Systems. *Journal of Physical Chemistry C*,	3.8	2
21	Stacking Order Effects on the Electronic and Optical Properties of Graphene/Transition Metal Dichalcogenide Van der Waals Heterostructures. *ACS Applied Electronic Materials*, **2021**, 3, 1671-1680	4	2
20	Excitonic Effects on Two-Dimensional Transition-Metal Dichalcogenide Monolayers: Impact on Solar Cell Efficiency. *ACS Applied Energy Materials*, **2021**, 4, 3265-3278	6.1	2
19	Energy Decomposition to Access the Stability Changes Induced by CO Adsorption on Transition-Metal 13-Atom Clusters. *Journal of Chemical Information and Modeling*, **2021**, 61, 2294-2301	6.1	2
18	Photomodulation of transport in monolayer dichalcogenides. *Physical Review B*, **2018**, 98,	3.3	2
17	Ab Initio Study of CO Activation on Pristine and Fe-Decorated WS Nanoflakes. *Journal of Physical Chemistry A*, **2021**, 125, 7769-7777	2.8	2
16	Ab initio investigation of the formation mechanism of nano-interfaces between 3d-late transition-metals and ZrO nanoclusters. *Physical Chemistry Chemical Physics*, **2020**, 22, 8067-8076	3.6	1
15	Tuning the optical bandgap in multi-cation compound transparent conducting-oxides: The examples of In2ZnO4 and In4Sn3O12. *Journal of Applied Physics*, **2018**, 123, 055704	2.5	1
14	Ab initio investigation of the role of charge transfer in the adsorption properties of H2, N2, O2,CO,NO,CO2, NO2, and CH4 on the van der Waals layered Sn3O4 semiconductor. *Physical Review Materials*, **2020**, 4,	3.2	1
13	A Hybrid Density Functional Theory Investigation of the (({text {CeO}}_2)_{6}) Clusters in the Cationic, Neutral, and Anionic States. *Journal of Cluster Science*, **2020**, 31, 1213-1220	3	1
12	An ab initio investigation of the adsorption properties of water on binary AlSi clusters. *Physical Chemistry Chemical Physics*, **2020**, 22, 24669-24676	3.6	1
11	Ab initio insights into the structural, energetic, electronic, and stability properties of mixed CeZrO nanoclusters. *Physical Chemistry Chemical Physics*, **2019**, 21, 26637-26646	3.6	1
10	Correlation-Based Framework for Extraction of Insights from Quantum Chemistry Databases: Applications for Nanoclusters. *Journal of Chemical Information and Modeling*, **2021**, 61, 1125-1135	6.1	1
9	Acid-base properties of hydroxyapatite(0001) by the adsorption of probe molecules: An ab initio investigation. *Physical Review Materials*, **2021**, 5,	3.2	1
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