Juarez L F Da Silva

List of Publications by Year in Descending Order

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	Role of quantum-size effects in the dehydrogenation of CH4 on 3d TMn clusters: DFT calculations combined with data mining. *Catalysis Science and Technology*, **2022**, 12, 916-926	5.5	
165	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
164	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
163	Ab initio investigation of the role of the d-states on the adsorption and activation properties of CO on 3d, 4d, and 5d transition-metal clusters.. *Journal of Chemical Physics*, **2022**, 156, 124106	3.9	
162	Tailoring Excitonic and Optoelectronic Properties of Transition Metal Dichalcogenide Bilayers. *Journal of Physical Chemistry C*, **2022**, 126, 9173-9184	3.8	1
161	Ab initio investigation of topological phase transitions induced by pressure in trilayer van der Waals structures: the example of h-BN/SnTe/h-BN. *Journal of Physics Condensed Matter*, **2021**, 33, 025003	1.8	0
160	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
159	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
158	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
157	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
156	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
155	Steric and Electrostatic Effects on the Diffusion of CH/CHOH in Copper-Exchanged Zeolites: Insights from Enhanced Sampling Molecular Dynamics and Free Energy Calculations. *Langmuir*, **2021**, 37, 8014-8023	4	0
154	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
153	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
152	Acid-base properties of hydroxyapatite(0001) by the adsorption of probe molecules: An ab initio investigation. *Physical Review Materials*, **2021**, 5,	3.2	1
151	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
150	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

149	Beyond the Anderson rule: importance of interfacial dipole and hybridization in van der Waals heterostructures. *2D Materials*, **2021**, 8, 041002	5.9	5
148	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
147	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
146	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
145	Role of the OH-group in the adsorption properties of methanol, ethanol, and ethylene glycol on 15-atom 3d, 4d, and 5d transition-metal clusters. *Physical Chemistry Chemical Physics*, **2021**, 23, 17553-17566	3.6	1
144	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
143	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
142	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
141	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
140	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
139	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
138	A hybrid-DFT investigation of the Ce oxidation state upon adsorption of F, Na, Ni, Pd and Pt on the (CeO) cluster. *Physical Chemistry Chemical Physics*, **2020**, 22, 14099-14108	3.6	5
137	Investigation of CO Adsorption on 13-Atom 4d Clusters. *Journal of Chemical Information and Modeling*, **2020**, 60, 537-545	6.1	11
136	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
135	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
134	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
133	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
132	Mixed Halide Lead-free Double Perovskite Alloys for Band Gap Engineering. *ACS Applied Energy Materials*, **2020**, 3, 7364-7371	6.1	3

131	Novel zero-dimensional lead-free bismuth based perovskites: from synthesis to structural and optoelectronic characterization. *Materials Advances*, **2020**, 1, 3439-3448	3.3	7
130	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
129	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
128	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
127	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
126	insights into the stabilization and binding mechanisms of MoS nanoflakes supported on graphene. *Physical Chemistry Chemical Physics*, **2020**, 22, 26865-26875	3.6	0
125	Defect-induced magnetism in II-VI quantum dots. *Physical Review B*, **2019**, 99,	3.3	2
124	(Meta-)stability and Core-Shell Dynamics of Gold Nanoclusters at Finite Temperature. *Journal of Physical Chemistry Letters*, **2019**, 10, 685-692	6.4	4
123	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
122	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
121	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
120	Edge, size, and shape effects on WS, WSe, and WTe nanoflake stability: design principles from an ab initio investigation. *Physical Chemistry Chemical Physics*, **2019**, 21, 23076-23084	3.6	11
119	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
118	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
117	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
116	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
115	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
114	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

113	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
112	Comparison of the Performance of van der Waals Dispersion Functionals in the Description of Water and Ethanol on Transition Metal Surfaces. *Journal of Physical Chemistry C*, **2018**, 122, 1577-1588	3.8	25
111	Ab Initio Investigation of the Role of Atomic Radius in the Structural Formation of PtnTM55−n (TM = Y, Zr, Nb, Mo, and Tc) Nanoclusters. *Journal of Physical Chemistry C*, **2018**, 122, 7444-7454	3.8	12
110	The role of the anionic and cationic pt sites in the adsorption site preference of water and ethanol on defected Pt4/Pt(111) substrates: A density functional theory investigation within the D3 van der waals corrections. *Surface Science*, **2018**, 667, 84-91	1.8	5
109	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
108	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
107	Size-Induced Phase Evolution of MoSe2 Nanoflakes Revealed by Density Functional Theory. *Journal of Physical Chemistry C*, **2018**, 122, 20483-20488	3.8	11
106	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
105	Water adsorption on the stoichiometric and defected Fe(110) surfaces. *Surface Science*, **2018**, 668, 144-149	1.8	11
104	Physical and Chemical Properties of Unsupported (MO2)n Clusters for M = Ti, Zr, or Ce and n = 1−15: 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
103	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
102	Photomodulation of transport in monolayer dichalcogenides. *Physical Review B*, **2018**, 98,	3.3	2
101	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
100	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
99	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
98	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
97	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
96	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

95	Glycerol adsorption on a defected Pt6/Pt(100) substrate: a density functional theory investigation within the D3 van der Waals correction. *RSC Advances*, **2017**, 7, 17122-17127	3.7	4
94	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
93	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
92	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
91	Interplay between structure asymmetry, defect-induced localization, and spin-orbit interaction in Mn-doped quantum dots. *Physical Review B*, **2017**, 95,	3.3	5
90	Graphene-supported small transition-metal clusters: A density functional theory investigation within van der Waals corrections. *Physical Review B*, **2017**, 95,	3.3	36
89	Stability and accuracy control of k □p parameters. *Semiconductor Science and Technology*, **2016**, 31, 105002	2.8	8
88	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
87	Electronic structure of layered quaternary chalcogenide materials for band-gap engineering: The example of Cs2MIIM3IVQ8. *Physical Review B*, **2016**, 93,	3.3	9
86	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
85	Nitroxyl as a ligand in ruthenium tetraammine systems: a density functional theory study. *Dalton Transactions*, **2016**, 45, 4907-15	4.3	6
84	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
83	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
82	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
81	A basin-hopping Monte Carlo investigation of the structural and energetic properties of 55- and 561-atom bimetallic nanoclusters: the examples of the ZrCu, ZrAl, and CuAl systems. *Journal of Physics Condensed Matter*, **2016**, 28, 175302	1.8	10
80	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
79	Structure, Electronic, and Magnetic Properties of Binary PtnTM55□ (TM = Fe, Co, Ni, Cu, Zn) Nanoclusters: A Density Functional Theory Investigation. *Journal of Physical Chemistry C*, **2015**, 119, 15669-15679	3.8	51
78	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

77	Comparative study of van der Waals corrections to the bulk properties of graphite. *Journal of Physics Condensed Matter*, **2015**, 27, 415502	1.8	32
76	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
75	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
74	Structural formation of binary PtCu clusters: A density functional theory investigation. *Computational Materials Science*, **2015**, 98, 278-286	3.2	34
73	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
72	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
71	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
70	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
69	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
68	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
67	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
66	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
65	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
64	Role of van der Waals corrections for the PtX2 (X=O, S, Se) compounds. *Physical Review B*, **2013**, 88,	3.3	23
63	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
62	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
61	Structural and electronic properties of TM23 - pAgp (TM = Ni, Pd, and Pt) clusters in the dilute limit (p = 0–4): A density functional theory investigation. *European Physical Journal D*, **2013**, 67, 1	1.3	13
60	Hybrid density functional study of small Rhn (n=2–15) clusters. *Physical Review B*, **2012**, 86,	3.3	32

59	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
58	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
57	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
56	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
55	Quantum Monte Carlo study of small aluminum clusters Aln (n=2−13). *Physical Review B*, **2012**, 85,	3.3	39
54	Multi-component transparent conducting oxides: progress in materials modelling. *Journal of Physics Condensed Matter*, **2011**, 23, 334210	1.8	39
53	Bulk structures of PtO and PtO2 from density functional calculations. *Physical Review B*, **2011**, 84,	3.3	29
52	Effective coordination concept applied for phase change (GeTe)m(Sb2Te3)n compounds. *Journal of Applied Physics*, **2011**, 109, 023502	2.5	72
51	Transition-metal 13-atom clusters assessed with solid and surface-biased functionals. *Journal of Chemical Physics*, **2011**, 134, 134105	3.9	24
50	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
49	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
48	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
47	Density functional theory investigation of 3d, 4d, and 5d 13-atom metal clusters. *Physical Review B*, **2010**, 81,	3.3	180
46	Electronic structure of In2O3 and Sn-doped In2O3 by hard x-ray photoemission spectroscopy. *Physical Review B*, **2010**, 81,	3.3	94
45	Reconstruction of core and surface nanoparticles: The example of Pt55 and Au55. *Physical Review B* , **2010**, 82,	3.3	50
44	Understanding the clean interface between covalent Si and ionic Al2O3. *Physical Review Letters*, **2009**, 103, 116101	7.4	20
43	Walsh, Da Silva, and Wei Reply:. *Physical Review Letters*, **2009**, 102,	7.4	7
42	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

41	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
40	Atomistic origins of the phase transition mechanism in Ge2Sb2Te5. *Journal of Applied Physics*, **2009**, 106, 113509	2.5	28
39	Ferrimagnetic Fe-doped GaN: An unusual magnetic phase in dilute magnetic semiconductors. *Physical Review B*, **2009**, 79,	3.3	24
38	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
37	Evidence for a subtle structural symmetry breaking in EuB(6). *Journal of Physics Condensed Matter*, **2009**, 21, 456007	1.8	6
36	Interplay between Order and Disorder in the High Performance of Amorphous Transparent Conducting Oxides. *Chemistry of Materials*, **2009**, 21, 5119-5124	9.6	80
35	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
34	Optical properties of pseudobinary GeTe, Ge2Sb2Te5, GeSb2Te4, GeSb4Te7, and Sb2Te3 from ellipsometry and density functional theory. *Physical Review B*, **2009**, 80,	3.3	110
33	Theoretical investigation of atomic and electronic structures of Ga2O3(ZnO)6. *Physical Review B*, **2009**, 80,	3.3	26
32	Trends in adsorption of noble gases He, Ne, Ar, Kr, and Xe on Pd(111)(3□)R30□ All-electron density-functional calculations. *Physical Review B*, **2008**, 77,	3.3	50
31	Origins of band-gap renormalization in degenerately doped semiconductors. *Physical Review B*, **2008**, 78,	3.3	235
30	Spin-orbit coupling and ion displacements in multiferroic TbMnO3. *Physical Review Letters*, **2008**, 101, 037209	7.4	158
29	Theoretical description of carrier mediated magnetism in cobalt doped ZnO. *Physical Review Letters* , **2008**, 100, 256401	7.4	240
28	Strain relaxation and band-gap tunability in ternary InxGa1□N nanowires. *Physical Review B*, **2008**, 78,	3.3	67
27	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
26	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
25	Rules of structure formation for the homologous InMO3(ZnO)n compounds. *Physical Review Letters* , **2008**, 100, 255501	7.4	59
24	Insights into the structure of the stable and metastable (GeTe)m(Sb2Te3)n compounds. *Physical Review B*, **2008**, 78,	3.3	147

23	Optical properties of (GeTe, Sb2Te3) pseudobinary thin films studied with spectroscopic ellipsometry. *Applied Physics Letters*, **2008**, 93, 021914	3.4	44
22	Effect of copassivation of Cl and Cu on CdTe grain boundaries. *Physical Review Letters*, **2008**, 101, 155501	7.4	95
21	Stability of the Ce2O3 phases: A DFT+U investigation. *Physical Review B*, **2007**, 76,	3.3	70
20	Formation of the cerium orthovanadate CeVO4: DFT+U study. *Physical Review B*, **2007**, 76,	3.3	56
19	Nature of Xenon adsorption on graphite: On-top versus hollow site preference. *Physical Review B*, **2007**, 76,	3.3	25
18	Atomic structure of In2O3□nO systems. *Applied Physics Letters*, **2007**, 90, 261904	3.4	30
17	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
16	Stability and electronic structures of CuxTe. *Applied Physics Letters*, **2007**, 91, 091902	3.4	54
15	Hybrid functionals applied to rare-earth oxides: The example of ceria. *Physical Review B*, **2007**, 75,	3.3	461
14	Converged properties of clean metal surfaces by all-electron first-principles calculations. *Surface Science*, **2006**, 600, 703-715	1.8	225
13	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
12	All-electron first-principles investigations of the energetics of vicinal Cu surfaces. *Physical Review B*, **2006**, 73,	3.3	48
11	Comment on □aming multiple valency with density functionals: A case study of defective ceria□ *Physical Review B*, **2005**, 72,	3.3	81
10	All-electron first-principles calculations of clean surface properties of low-Miller-index Al surfaces. *Physical Review B*, **2005**, 71,	3.3	51
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