Javier Fernndez Sanz

List of Publications by Citations

208 papers	7,779 citations	44 h-index	81 g-index
216 ext. papers	8,304 ext. citations	5.2 avg, IF	5.82 L-index

#	Paper	IF	Citations
208	Catalysis. Highly active copper-ceria and copper-ceria-titania catalysts for methanol synthesis from CO. *Science*, **2014**, 345, 546-50	33.3	895
207	Importance of the metal-oxide interface in catalysis: in situ studies of the water-gas shift reaction by ambient-pressure X-ray photoelectron spectroscopy. *Angewandte Chemie - International Edition*, **2013**, 52, 5101-5	16.4	245
206	High catalytic activity of Au/CeOx/TiO2(110) controlled by the nature of the mixed-metal oxide at the nanometer level. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 4975-80	11.5	241
205	Gold, copper, and platinum nanoparticles dispersed on CeO(x)/TiO(2)(110) surfaces: high water-gas shift activity and the nature of the mixed-metal oxide at the nanometer level. *Journal of the American Chemical Society*, **2010**, 132, 356-63	16.4	232
204	Water-gas shift reaction on a highly active inverse CeOx/Cu111 catalyst: unique role of ceria nanoparticles. *Angewandte Chemie - International Edition*, **2009**, 48, 8047-50	16.4	228
203	High Water-Gas Shift Activity in TiO2(110) Supported Cu and Au Nanoparticles: Role of the Oxide and Metal Particle Size. *Journal of Physical Chemistry C*, **2009**, 113, 7364-7370	3.8	211
202	CO oxidation on inverse CeO(x)/Cu(111) catalysts: high catalytic activity and ceria-promoted dissociation of O2. *Journal of the American Chemical Society*, **2011**, 133, 3444-51	16.4	207
201	Coumarin derivatives for dye sensitized solar cells: a TD-DFT study. *Physical Chemistry Chemical Physics*, **2012**, 14, 225-33	3.6	157
200	Effect of on-site Coulomb repulsion term U on the band-gap states of the reduced rutile (110) TiO2 surface. *Physical Review B*, **2008**, 77,	3.3	153
199	Real-Time TD-DFT Simulations in Dye Sensitized Solar Cells: The Electronic Absorption Spectrum of Alizarin Supported on TiO2 Nanoclusters. *Journal of Chemical Theory and Computation*, **2010**, 6, 2856-65	6.4	142
198	N doping of TiO2(110): photoemission and density-functional studies. *Journal of Chemical Physics*, **2006**, 125, 094706	3.9	122
197	Frequency dependent hyperpolarizabilities with application to formaldehyde and methyl fluoride. *Journal of Chemical Physics*, **1990**, 93, 8828-8839	3.9	121
196	Cu, Ag, and Au atoms adsorbed on TiO2(110): cluster and periodic calculations. *Surface Science*, **2001**, 471, 21-31	1.8	117
195	Direct vs Indirect Mechanisms for Electron Injection in Dye-Sensitized Solar Cells. *Journal of Physical Chemistry C*, **2011**, 115, 11293-11301	3.8	110
194	Au N synergy and N-doping of metal oxide-based photocatalysts. *Journal of the American Chemical Society*, **2008**, 130, 12056-63	16.4	110
193	Comparative Study on the Performance of Hybrid DFT Functionals in Highly Correlated Oxides: The Case of CeO2 and Ce2O3. *Journal of Chemical Theory and Computation*, **2011**, 7, 56-65	6.4	108
192	Density Functional Theory Study of the Interaction of Cu, Ag, and Au Atoms with the Regular CeO2 (111) Surface. *Journal of Physical Chemistry C*, **2010**, 114, 1934-1941	3.8	103

191	N Doping of Rutile TiO2 (110) Surface. A Theoretical DFT Study. *Journal of Physical Chemistry C*, **2008**, 112, 2624-2631	3.8	100
190	Methanol Adsorption and Dissociation on TiO2(110) from First Principles Calculations. *Journal of Physical Chemistry C*, **2007**, 111, 10023-10028	3.8	95
189	Electronic structure and optical spectra of catechol on TiO2 nanoparticles from real time TD-DFT simulations. *Physical Chemistry Chemical Physics*, **2011**, 13, 1506-14	3.6	90
188	Methanol and Water Dissociation on TiO2 (110): The Role of Surface Oxygen. *Journal of Physical Chemistry C*, **2008**, 112, 17737-17740	3.8	89
187	On modelling the interaction of CO on the MgO(100) surface. *Surface Science*, **1995**, 327, 59-73	1.8	87
186	Inverse Oxide/Metal Catalysts in Fundamental Studies and Practical Applications: A Perspective of Recent Developments. *Journal of Physical Chemistry Letters*, **2016**, 7, 2627-39	6.4	86
185	A theoretical insight into the catalytic effect of a mixed-metal oxide at the nanometer level: the case of the highly active metal/CeOx/TiO2(110) catalysts. *Journal of Chemical Physics*, **2010**, 132, 104703	3.9	85
184	Accurate ab initio determination of magnetic interactions and hopping integrals in La2-xSrxCuO4 systems. *Journal of Chemical Physics*, **2000**, 112, 5158-5167	3.9	84
183	Electronic charge transfer between ceria surfaces and gold adatoms: a GGA+U investigation. *Physical Chemistry Chemical Physics*, **2009**, 11, 5246-52	3.6	78
182	Graphenes as Efficient Metal-Free Fenton Catalysts. *Chemistry - A European Journal*, **2015**, 21, 11966-71	4.8	73
181	Oxygen vacancies on TiO2 (110) from first principles calculations. *Journal of Chemical Physics*, **2004**, 121, 7427-33	3.9	67
180	Unravelling the origin of the high-catalytic activity of supported Au: a density-functional theory-based interpretation. *Journal of the American Chemical Society*, **2006**, 128, 15600-1	16.4	65
179	Visible Light-Driven H2 Production over Highly Dispersed Ruthenia on Rutile TiO2 Nanorods. *ACS Catalysis*, **2016**, 6, 407-417	13.1	63
178	First-principles calculations of structural and electronic properties of monoclinic hafnia surfaces. *Physical Review B*, **2006**, 73,	3.3	63
177	Nature of the Mixed-Oxide Interface in Ceria-Titania Catalysts: Clusters, Chains, and Nanoparticles. *Journal of Physical Chemistry C*, **2013**, 117, 14463-14471	3.8	62
176	V@Au12-: an improved novel catalyst for CO oxidation?. *Journal of Physical Chemistry B*, **2006**, 110, 11600-3	3.4	60
175	Electron Mobility via Polaron Hopping in Bulk Ceria: A First-Principles Study. *Journal of Physical Chemistry C*, **2013**, 117, 14502-14509	3.8	59
174	On the difficulties of present theoretical models to predict the oxidation state of atomic Au adsorbed on regular sites of CeO2(111). *Journal of Chemical Physics*, **2009**, 131, 094702	3.9	58

173	Cu, Ag and Au atoms deposited on the α-Al2O3(0001) surface: a comparative density functional study. *Surface Science*, **2005**, 575, 189-196	1.8	55
172	Communication: improving the density functional theory+U description of CeO2 by including the contribution of the O 2p electrons. *Journal of Chemical Physics*, **2012**, 136, 041101	3.9	54
171	Theoretical Investigation of the Deposition of Cu, Ag, and Au Atoms on the ZrO2(111) Surface. *Journal of Physical Chemistry C*, **2007**, 111, 10448-10454	3.8	54
170	Interaction of Pd with α-Al2O3(0001): A case study of modeling the metal-oxide interface on complex substrates. *Physical Review B*, **2002**, 65,	3.3	50
169	Molecular dynamics studies of the structure of α-alumina. *Chemical Physics Letters*, **1992**, 192, 463-468	2.5	49
168	Adsorption of Pd Atoms and Dimers on the TiO2(110) Surface: A First Principles Study. *Journal of Physical Chemistry C*, **2007**, 111, 3949-3955	3.8	48
167	Determining the behavior of RuO(x) nanoparticles in mixed-metal oxides: structural and catalytic properties of RuO2/TiO2(110) surfaces. *Angewandte Chemie - International Edition*, **2011**, 50, 10198-202	16.4	47
166	Ab initio systematic determination of the t-J effective Hamiltonian parameters for superconducting Cu-oxides. *Chemical Physics Letters*, **1999**, 307, 102-108	2.5	46
165	Molecular-dynamics simulations of liquid aluminum oxide. *Physical Review B*, **1998**, 58, 2369-2371	3.3	45
164	Role of vacancies in the structural stability of TiO: A first-principles study based on density-functional calculations. *Physical Review B*, **2005**, 72,	3.3	44
163	Surface model and exchange-correlation functional effects on the description of Pd/α-Al2O3(0001). *Journal of Chemical Physics*, **2002**, 116, 1684-1691	3.9	44
162	Sonogashira cross-coupling and homocoupling on a silver surface: chlorobenzene and phenylacetylene on Ag(100). *Journal of the American Chemical Society*, **2015**, 137, 940-7	16.4	43
161	Molecular-dynamics simulations of (NaO2)x(SiO2)1-x glasses: Relation between distribution and diffusive behavior of Na atoms. *Physical Review B*, **1998**, 58, 9047-9053	3.3	43
160	Effect of dispersion correction on the Au(1 1 1)-H2O interface: a first-principles study. *Journal of Chemical Physics*, **2012**, 137, 114709	3.9	42
159	Interaction of oxygen with TiN(001): NO exchange and oxidation process. *Journal of Chemical Physics*, **2007**, 126, 244713	3.9	42
158	Computer Simulation of .gamma.-Al2O3 Microcrystal. *The Journal of Physical Chemistry*, **1995**, 99, 17872-17876		42
157	Direct vs. indirect mechanisms for electron injection in DSSC: Catechol and alizarin. *Computational and Theoretical Chemistry*, **2011**, 975, 99-105	2	41
156	Electronic structure of the transition-metal-carbene-like complexes (CO)5Mo-MNH2 (MN= carbon, silicon, germanium and tin). A theoretical study based on ab initio CASSCF calculations. *Journal of the American Chemical Society*, **1992**, 114, 2903-2909	16.4	40

155	Drifts, XPS, XAS, and ab Initio Study of Lanthanide Oxides Supported on .gamma.-Al2O3. *The Journal of Physical Chemistry*, **1995**, 99, 4655-4660		39
154	Surface models for Al2O3 from molecular dynamics simulations. *Journal of the Chemical Society, Faraday Transactions*, **1993**, 89, 3623-3628		39
153	Surface structure of cubic aluminum oxide. *Physical Review B*, **1994**, 50, 2561-2565	3.3	39
152	Transport Properties in the CeO2(111) Surface: From Charge Distribution to Ion-Electron Collaborative Migration. *Journal of Physical Chemistry C*, **2013**, 117, 25497-25503	3.8	38
151	Atomic layer deposition of hafnium oxide from hafnium chloride and water. *Journal of the American Chemical Society*, **2008**, 130, 11996-2006	16.4	37
150	N2O decomposition on TiO2 (110) from dynamic first-principles calculations. *Journal of Physical Chemistry B*, **2005**, 109, 16223-6	3.4	37
149	Carbon Doping of the TiO2 (110) Rutile Surface. A Theoretical Study Based on DFT. *Chemistry of Materials*, **2009**, 21, 1431-1438	9.6	36
148	Changing the physical and chemical properties of titanium oxynitrides TiN1Ox by changing the composition. *Physical Review B*, **2009**, 80,	3.3	36
147	Molecular dynamics simulations of Na deposition on the TiO2(110) surface. *Surface Science*, **1998**, 409, 92-100	1.8	35
146	Mechanism of Cu deposition on the alpha-Al(2)O(3) (0001) surface. *Physical Review Letters*, **2005**, 94, 016104	7.4	35
145	Compact model potentials for ab initio embedded cluster calculations. Part I. Basic formulation. *Journal of Chemical Physics*, **1995**, 102, 327-336	3.9	35
144	Theoretical calculations of proton affinities of azines. Prediction of the relative basicities and preferred protonation sites. *Journal of Computational Chemistry*, **1988**, 9, 784-789	3.5	35
143	Nitrogen/gold codoping of the TiO2(101) anatase surface. A theoretical study based on DFT calculations. *Physical Chemistry Chemical Physics*, **2011**, 13, 11340-50	3.6	34
142	Cu Deposited on CeOx-Modified TiO2(110): Synergistic Effects at the Metal–Oxide Interface and the Mechanism of the WGS Reaction. *ACS Catalysis*, **2016**, 6, 4608-4615	13.1	33
141	Synthesis, solid-state structure, and bonding analysis of the beryllocenes [Be(C5Me4H)2], [Be(C5Me5)2], and [Be(C5Me5)(C5Me4H)]. *Chemistry - A European Journal*, **2003**, 9, 4452-61	4.8	32
140	Direct determination of the effective electronic coupling in electron-transfer problems. *The Journal of Physical Chemistry*, **1993**, 97, 99-106		32
139	Structural Defects in W-Doped TiO2 (101) Anatase Surface: Density Functional Study. *Journal of Physical Chemistry C*, **2011**, 115, 16970-16976	3.8	31
138	First Principles Study of Cu Atoms Deposited on the Al2O3(0001) Surface. *Journal of Physical Chemistry B*, **2002**, 106, 11495-11500	3.4	31

137	Spectroscopic properties and potential energy curves of some low-lying electronic states of AlO, AlO+, LaO, and LaO+: An ab initio CASSCF study. *International Journal of Quantum Chemistry*, **1994**, 52, 1329-1338	2.1	30
136	Molecular modification of coumarin dyes for more efficient dye sensitized solar cells. *Journal of Chemical Physics*, **2012**, 136, 194702	3.9	29
135	Density Functional Theory Study of Co, Rh, and Ir Atoms Deposited on the □Al2O3(0001) Surface. *Journal of Physical Chemistry B*, **2004**, 108, 15671-15678	3.4	29
134	Designing a new generation of catalysts: Water gas shift reaction example. *Catalysis Today*, **2015**, 240, 214-219	5.3	28
133	Unraveling the Nature of the Oxide□Metal Interaction in Ceria-Based Noble Metal Inverse Catalysts. *Journal of Physical Chemistry C*, **2014**, 118, 26931-26938	3.8	27
132	The Flexible Surface Revisited: Adsorbate-Induced Reconstruction, Homocoupling, and Sonogashira Cross-Coupling on the Au(100) Surface. *Journal of Physical Chemistry C*, **2014**, 118, 11677-11684	3.8	27
131	Simulating the optical properties of CdSe clusters using the RT-TDDFT approach. *Theoretical Chemistry Accounts*, **2013**, 132, 1	1.9	27
130	Structural, electronic and optical properties of copper, silver and gold sulfide: a DFT study. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	26
129	First-Principles Investigation of Hydroxylated Monoclinic HfO2 Surfaces. *Chemistry of Materials*, **2006**, 18, 3397-3403	9.6	26
128	Supramolecular interactions as determining factors of the geometry of metallic building blocks: tetracarboxylate dimanganese species. *Angewandte Chemie - International Edition*, **2005**, 44, 3429-32	16.4	26
127	Making Photo-selective TiO2 Materials by Cation□Anion Codoping: From Structure and Electronic Properties to Photoactivity. *Journal of Physical Chemistry C*, **2012**, 116, 18759-18767	3.8	25
126	Gold Nanoparticles on Yttrium Modified Titania: Support Properties and Catalytic Activity. *Topics in Catalysis*, **2011**, 54, 219-228	2.3	24
125	Thiodiacetate-manganese chemistry with N ligands: unique control of the supramolecular arrangement over the metal coordination mode. *Chemistry - A European Journal*, **2011**, 17, 10600-17	4.8	24
124	Molecular Dynamics Simulations of the Structure of Pd Clusters Deposited on the MgO(001) Surface. *Journal of Physical Chemistry B*, **2000**, 104, 4342-4348	3.4	24
123	Molecular Dynamics Simulations of Pd Deposition on the □Al2O3 (0001) Surface. *Journal of Physical Chemistry B*, **2001**, 105, 12111-12117	3.4	24
122	Surface oxygen vacancies in gold based catalysts for CO oxidation. *RSC Advances*, **2014**, 4, 13145-13152	3.7	23
121	Role of Coverage and Surface Oxidation Degree in the Adsorption of Acetone on TiO2 (110). A Density Functional Study. *Journal of Physical Chemistry C*, **2009**, 113, 19973-19980	3.8	22
120	The vacuum-ultraviolet spectrum of iron pentacarbonyl: An experimental analysis supported by a CASSCF CCI study of the Rydberg states. *The Journal of Physical Chemistry*, **1992**, 96, 121-123		22

119	Theoretical Analysis of K Adsorption on TiO2(110) Rutile Surface. *Journal of Physical Chemistry B*, **1999**, 103, 480-486	3.4	21
118	Water□Gas Shift Reaction on K/Cu(111) and Cu/K/TiO2(110) Surfaces: Alkali Promotion of Water Dissociation and Production of H2. *ACS Catalysis*, **2019**, 9, 10751-10760	13.1	20
117	Understanding Acetaldehyde Thermal Chemistry on the TiO2 (110) Rutile Surface: From Adsorption to Reactivity. *Journal of Physical Chemistry C*, **2011**, 115, 2819-2825	3.8	20
116	Adsorption of Pd atoms on □Al2O3: a density functional study of metal□support interactions. *Applied Surface Science*, **2004**, 238, 82-85	6.7	20
115	Reactions of {[Pd(&mgr;-SC(6)F(5))(&mgr;-dppm)Pd](&mgr;-SC(6)F(5))}(4).2O(C(2)H(5))(2). Crystal Structures of the Complexes [(Ph(3)P)Pd(&mgr;-SC(6)F(5))(&mgr;-dppm)Pd(SC(6)F(5))].1.4CH(2)Cl(2) and [(Ph(3)P)Pd(&mgr;-SC(6)F(5))(&mgr;-dppm)Pd(PPh(3))]SO(3)CF(3).2CH(2)Cl(2) and ab Initio MO Calculations on the Model Systems [(H(3)P)Pd(&mgr;-H(2)PCH(2)PH(2))(&mgr;-SH)Pd(PH(3))](+) and [(H(3)P)Pd(&mgr;-H(2)PCH(2)PH(2))Pd(PH(3))](2+). *Inorganic Chemistry*, **1997**, 36, 1912-1922	5.1	19
114	Dedicated Molecular Orbitals for the Variational Determination of the Electron-Transfer Matrix Element. Method and Application to a Cu(I)□Cu(II) Mixed Valence Compound. *Journal of Physical Chemistry A*, **1997**, 101, 1716-1721	2.8	19
113	Physical Factors Governing the Amplitude of the Electron Transfer Integral in Mixed-Valence Compounds. *Journal of Physical Chemistry A*, **1998**, 102, 3659-3667	2.8	19
112	Adsorption of Acetone onto MgO: Experimental and Theoretical Evidence for the Presence of a Surface Enolate. *Angewandte Chemie - International Edition*, **1999**, 38, 506-509	16.4	19
111	Solvent effects on the dissociation of aliphatic carboxylic acids in water□N,N -dimethylformamide mixtures. *Analytica Chimica Acta*, **1990**, 228, 301-306	6.6	19
110	First principles simulations of Cu and Au deposition on □Al2O3 (0 0 0 1) surface. *Applied Surface Science*, **2004**, 238, 228-232	6.7	18
109	First-principles molecular dynamics simulations of the H2O/Cu(111) interface. *Journal of Molecular Modeling*, **2012**, 18, 2433-42	2	17
108	First principles study of Na adsorption on TiO2 (110) surface. *International Journal of Quantum Chemistry*, **1998**, 70, 351-357	2.1	17
107	Theoretical models for □Al2O3 (110) surface hydroxylation: An ab initio embedded cluster study. *International Journal of Quantum Chemistry*, **1998**, 70, 359-365	2.1	17
106	Geometric and Electronic Structure of Amorphous Aluminophosphates. Ab Initio and Experimental Studies. *Journal of Physical Chemistry B*, **1997**, 101, 9510-9516	3.4	16
105	Understanding the Interplay of Dopants, Interfaces, and Anionic Conductivity in Doped Ceria/Zirconia Heteroepitaxial Structures. *Chemistry of Materials*, **2014**, 26, 3385-3390	9.6	15
104	Relaxation of the (001) surface in binary Sc, Ti and V nitrides: a first principles density functional study. *Surface Science*, **2003**, 541, 217-224	1.8	15
103	Ab Initio Calculations of the Electron-Transfer Matrix Element in CuI□CuII Mixed-Valence Compounds. *Journal of the American Chemical Society*, **1998**, 120, 1051-1061	16.4	15
102	Molecular dynamics simulations of the MgO(001) surface hydroxylation. *Journal of Chemical Physics* , **1998**, 108, 4219-4225	3.9	15

101	A periodic Hartree–Fock study of Na adsorption on the TiO2(110) rutile surface. *Chemical Physics Letters*, **1999**, 303, 111-116	2.5	15
100	Ab initio CASSCF study of the electronic structure of the transition-metal alkylidene-like complexes Mo-MNH2 (MN= carbon, silicon, germanium and tin). *Journal of the American Chemical Society*, **1992**, 114, 10019-10024	16.4	15
99	AgS Quantum Dot-Sensitized Solar Cells by First Principles: The Effect of Capping Ligands and Linkers. *Journal of Physical Chemistry A*, **2017**, 121, 7290-7296	2.8	14
98	Effect of capping ligands and TiO2 supporting on the optical properties of a (CdSe)13 cluster. *Journal of Physical Chemistry A*, **2015**, 119, 1218-27	2.8	14
97	Ab initio CI calculations on the molecular structure of Sn2H4 isomers. *Chemical Physics*, **1989**, 138, 99-104	2.3	14
96	Adsorption of Prototypical Asphaltenes on Silica: First-Principles DFT Simulations Including Dispersion Corrections. *Journal of Physical Chemistry B*, **2018**, 122, 618-624	3.4	14
95	Charge state of metal atoms on oxide supports: a systematic study based on simulated infrared spectroscopy and density functional theory. *Theoretical Chemistry Accounts*, **2010**, 126, 265-273	1.9	13
94	Parallel computation of second derivatives of RHF energy on distributed memory computers. *Journal of Computational Chemistry*, **1997**, 18, 159-168	3.5	13
93	Synthesis, Structural Characterization, and MO Calculations of Vanadium Imido Complexes Containing Bidentate Phosphine Coligands. *Inorganic Chemistry*, **1999**, 38, 4462-4466	5.1	13
92	Potassium and Water Coadsorption on TiO(110): OH-Induced Anchoring of Potassium and the Generation of Single-Site Catalysts. *Journal of Physical Chemistry Letters*, **2016**, 7, 3866-3872	6.4	12
91	A Density Functional Study of Initial Steps in the Oxidation of Early Transition Metal Nitrides, MN (M = Sc, Ti, and V). *Journal of Physical Chemistry C*, **2009**, 113, 930-938	3.8	12
90	DFT versus CI determination of the electron-transfer matrix element in some case examples. *International Journal of Quantum Chemistry*, **2000**, 76, 458-463	2.1	12
89	Cr2O3 (0001) oxygen-terminating surface. A molecular dynamics study. *Computational and Theoretical Chemistry*, **1999**, 463, 185-190		12
88	Unrestricted compact model potentials for ab initio embedded cluster calculations: Magnetic interactions in KNiF3. *Journal of Chemical Physics*, **1995**, 102, 850-858	3.9	12
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82	Redox properties of gold-substituted zirconia surfaces. *Journal of Materials Chemistry*, **2009**, 19, 710-717		11
81	The thermostabilising effect of La doping on Al2O3 a molecular dynamics simulation study. *Solid State Ionics*, **1997**, 95, 73-79	3.3	11
80	Ab initio study of the adsorption of acetone and keto-enol equilibrium on the MgO(100) surface. *Surface Science*, **1998**, 397, 23-33	1.8	11
79	Influence of temperature on the interaction between Pd clusters and the TiO2 (110) surface. *Physical Review Letters*, **2007**, 99, 066102	7.4	11
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75	Comprehensive Experimental and Theoretical Study of the CO + NO Reaction Catalyzed by Au/Ni Nanoparticles. *ACS Catalysis*, **2019**, 9, 4919-4929	13.1	10
74	Coverage and charge dependent adsorption of butanethiol on the Au(111) surface: A density functional theory study. *Computational and Theoretical Chemistry*, **2011**, 975, 116-121	2	10
73	A theoretical study of the Na?TiO2 (001) rutile interaction. *Journal of Molecular Catalysis A*, **1997**, 119, 135-142		10
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71	Theoretical Approach to Ionic Conductivity in PhosphorusOxynitride Compounds. *Journal of Solid State Chemistry*, **2001**, 161, 73-79	3.3	10
70	A first principles study of Pd deposition on the TiO2(1 1 0) surface. *Theoretical Chemistry Accounts*, **2000**, 104, 317-322	1.9	10
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68	Ab initio calculations of molecular and electronic structure of disilane. I. Molecular force field and vibrational spectrum. *Chemical Physics*, **1991**, 149, 311-318	2.3	10
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66	Photo-sensitizing thin-film ferroelectric oxides using materials databases and high-throughput calculations. *Journal of Materials Chemistry A*, **2019**, 7, 27323-27333	13	10

65	Graphene Translucency and Interfacial Interactions in the Gold/Graphene/SiC System. *Journal of Physical Chemistry Letters*, **2018**, 9, 3850-3855	6.4	10
64	Experimental and molecular dynamics simulation analysis of LaCrO3 precipitation in chromia scales. *Acta Materialia*, **2000**, 48, 2951-2958	8.4	9
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