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List of Publications by Year
in descending order

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84 papers	2,252 citations	201674 27 h-index	243625 44 g-index
89 all docs	89 docs citations	89 times ranked	2852 citing authors

#	Article	IF	Citations
1	Comparative Study on the Performance of Hybrid DFT Functionals in Highly Correlated Oxides: The Case of CeO₂and Ce₂O₃. Journal of Chemical Theory and Computation, 2011, 7, 56-65.	5.3	125
2	Optical Absorption and Nonradiative Decay Mechanism ofEâ€²Center in Silica. Physical Review Letters, 1998, 81, 377-380.	7.8	113
3	Electronic structure and optical spectra of catechol on TiO₂nanoparticles from real time TD-DFT simulations. Physical Chemistry Chemical Physics, 2011, 13, 1506-1514.	2.8	103
4	A CSOV study of the difference between HF and DFT intermolecular interaction energy values: The importance of the charge transfer contribution. Journal of Computational Chemistry, 2005, 26, 1052-1062.	3.3	99
5	On modelling the interaction of CO on the MgO(100) surface. Surface Science, 1995, 327, 59-73.	1.9	96
6	Importance of Madelung potential in quantum chemical modeling of ionic surfaces. Journal of Computational Chemistry, 1997, 18, 617-628.	3.3	85
7	Electron Mobility via Polaron Hopping in Bulk Ceria: A First-Principles Study. Journal of Physical Chemistry C, 2013, 117, 14502-14509.	3.1	75
8	Origin of the vibrational shift of CO chemisorbed on Pt(111). Physical Review B, 1995, 52, 12372-12379.	3.2	65
9	Cu, Ag and Au atoms deposited on the Î±-Al2O3(0001) surface: a comparative density functional study. Surface Science, 2005, 575, 189-196.	1.9	63
10	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.	3.0	62
11	On the bonding mechanism of CO to Pt(111) and its effect on the vibrational frequency of chemisorbed CO. Surface Science, 1997, 376, 279-296.	1.9	61
12	Adsorption of Pd Atoms and Dimers on the TiO2(110) Surface:â€‰ A First Principles Study. Journal of Physical Chemistry C, 2007, 111, 3949-3955.	3.1	51
13	Role of vacancies in the structural stability ofÎ±â^'TiO: A first-principles study based on density-functional calculations. Physical Review B, 2005, 72, .	3.2	50
14	Electronic structure of the transition-metal-carbene-like complexes (CO)5Mo-M'H2 (M' = carbon,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 American Chemical Society, 1992, 114, 2903-2909.	13.7	46
15	A DFT Theoretical Analysis of Aldehyde Condensation Pathways onto Methyllithium, Lithium Dimethylamide, and Their Aggregates. Journal of Organic Chemistry, 2000, 65, 8899-8907.	3.2	45
16	Transport Properties in the CeO_{2â€“x}(111) Surface: From Charge Distribution to Ion-Electron Collaborative Migration. Journal of Physical Chemistry C, 2013, 117, 25497-25503.	3.1	41
17	Similarities and differences in the Hartreeâ€“Fock and density-functional description of the chemisorption bond. Surface Science, 1999, 442, 463-476.	1.9	37
18	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, 4452-4461.	3.3	37

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19	The Rys quadrature revisited: A novel formulation for the efficient computation of electron repulsion integrals over Gaussian functions. Journal of Chemical Physics, 2001, 114, 2067-2078.	3.0	35
20	Modeling of Copper(II) Complexes with the SIBFA Polarizable Molecular Mechanics Procedure. Application to a New Class of HIV-1 Protease Inhibitors. Journal of Physical Chemistry B, 2003, 107, 10640-10652.	2.6	35
21	Structural, electronic and optical properties of copper, silver and gold sulfide: a DFT study. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	35
22	Structural Defects in W-Doped TiO₂ (101) Anatase Surface: Density Functional Study. Journal of Physical Chemistry C, 2011, 115, 16970-16976.	3.1	34
23	Spectroscopic properties and potential energy curves of some low-lying electronic states of AlO, AlO+, LaO, and LaO+: An ab initioCASSCFstudy. International Journal of Quantum Chemistry, 1994, 52, 1329-1338.	2.0	33
24	Density Functional Theory Study of Co, Rh, and Ir Atoms Deposited on the Î±-Al2O3(0001) Surface. Journal of Physical Chemistry B, 2004, 108, 15671-15678.	2.6	30
25	Parallel computation of the MP2 energy on distributed memory computers. Journal of Computational Chemistry, 1995, 16, 395-404.	3.3	29
26	Making Photo-selective TiO₂ Materials by Cationâ€“Anion Codoping: From Structure and Electronic Properties to Photoactivity. Journal of Physical Chemistry C, 2012, 116, 18759-18767.	3.1	29
27	Valence contrast by synchrotron resonance scattering: application to a mixed-valence manganese compound. Journal of the American Chemical Society, 1992, 114, 9214-9215.	13.7	28
28	Analysis of electronic contributions to the vibrational frequency of CO/Cu2O(111). Surface Science, 1999, 430, 137-145.	1.9	28
29	Gold Nanoparticles on Yttrium Modified Titania: Support Properties and Catalytic Activity. Topics in Catalysis, 2011, 54, 219-228.	2.8	25
30	Adsorption of Acetone onto MgO: Experimental and Theoretical Evidence for the Presence of a Surface Enolate. Angewandte Chemie - International Edition, 1999, 38, 506-509.	13.8	24
31	The Effect of Pyrimidine Bases on the Hole-Transfer Coupling in DNAâ€. Journal of Physical Chemistry B, 2002, 106, 7919-7926.	2.6	24
32	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.	3.1	24
33	Surface oxygen vacancies in gold based catalysts for CO oxidation. RSC Advances, 2014, 4, 13145-13152.	3.6	24
34	Adsorption of Pd atoms on Î³-Al2O3: a density functional study of metalâ€“support interactions. Applied Surface Science, 2004, 238, 82-85.	6.1	23
35	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.	2.9	22
36	Understanding Acetaldehyde Thermal Chemistry on the TiO₂ (110) Rutile Surface: From Adsorption to Reactivity. Journal of Physical Chemistry C, 2011, 115, 2819-2825.	3.1	22

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37	Comprehensive Experimental and Theoretical Study of the CO + NO Reaction Catalyzed by Au/Ni Nanoparticles. ACS Catalysis, 2019, 9, 4919-4929.	11.2	22
38	Charting the Lattice Thermal Conductivities of Iâ€“IIIâ€“VI₂ Chalcopyrite Semiconductors. Chemistry of Materials, 2022, 34, 2833-2841.	6.7	22
39	Adsorption of Prototypical Asphaltenes on Silica: First-Principles DFT Simulations Including Dispersion Corrections. Journal of Physical Chemistry B, 2018, 122, 618-624.	2.6	21
40	Ab initio CASSCF study of the electronic structure of the transition-metal alkylidene-like complexes Mo-M'H2 (M' = carbon, silicon, germanium and tin). Journal of the American Chemical Society, 1992, 114, 10019-10024.	13.7	20
41	Theoretical values of the enthalpies of formation of the NHx (x = 1,2,3) compounds. Importance of the core-correlation effects. Chemical Physics Letters, 1995, 233, 220-226.	2.6	20
42	Theoretical models for ?-Al2O3 (110) surface hydroxylation: An ab initio embedded cluster study. International Journal of Quantum Chemistry, 1998, 70, 359-365.	2.0	20
43	Host-guest interactions between cyclodextrins and surfactants with functional groups at the end of the hydrophobic tail. Journal of Colloid and Interface Science, 2017, 491, 336-348.	9.4	19
44	Ab initio CI calculations on the molecular structure of Sn2H4 isomers. Chemical Physics, 1989, 138, 99-104.	1.9	18
45	Geometric and Electronic Structure of Amorphous Aluminophosphates. Ab Initio and Experimental Studies. Journal of Physical Chemistry B, 1997, 101, 9510-9516.	2.6	18
46	Theoretical enthalpy of formation of the acetonyl radical. Chemical Physics Letters, 2003, 373, 350-356.	2.6	17
47	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.	1.4	17
48	Ag₂S Quantum Dot-Sensitized Solar Cells by First Principles: The Effect of Capping Ligands and Linkers. Journal of Physical Chemistry A, 2017, 121, 7290-7296.	2.5	17
49	Understanding the Interplay of Dopants, Interfaces, and Anionic Conductivity in Doped Ceria/Zirconia Heteroepitaxial Structures. Chemistry of Materials, 2014, 26, 3385-3390.	6.7	16
50	Molecular dynamics simulations of the role of salinity and temperature on the hydrocarbon/water interfacial tension. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	16
51	Parallel computation of second derivatives of RHF energy on distributed memory computers. Journal of Computational Chemistry, 1997, 18, 159-168.	3.3	15
52	Ab Initio SCF-Mo Study of the Chemisorption of Methane on Al and La Oxide Surfaces. Journal of Catalysis, 1995, 156, 273-278.	6.2	14
53	DFTversus CI determination of the electron-transfer matrix element in some case examples. International Journal of Quantum Chemistry, 2000, 76, 458-463.	2.0	12
54	A Density Functional Study of Initial Steps in the Oxidation of Early Transition Metal Nitrides, MN (M =) Tj ETQq0 0 0 rgBT /Overlock 10 T	3.1	12

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55	Effects of the capping ligands, linkers and oxide surface on the electron injection mechanism of copper sulfide quantum dot-sensitized solar cells. Physical Chemistry Chemical Physics, 2017, 19, 14580-14587.	2.8	12
56	Photo-sensitizing thin-film ferroelectric oxides using materials databases and high-throughput calculations. Journal of Materials Chemistry A, 2019, 7, 27323-27333.	10.3	12
57	Ab initio calculations of molecular and electronic structure of disilane. I. Molecular force field and vibrational spectrum. Chemical Physics, 1991, 149, 311-318.	1.9	11
58	A first principles study of Pd deposition on the TiO 2 (1 1 0) surface. Theoretical Chemistry Accounts, 2000, 104, 317-322.	1.4	11
59	Adsorption of prototypical amino acids on silica: Influence of the pre-adsorbed water multilayer. Surface Science, 2016, 646, 239-246.	1.9	10
60	A Theoretical Study of ZnCH2 and ZnSnH2 Electronic Structure and the ZnCH2â˜HZnCH Photolytic Rearrangement. Journal of the American Chemical Society, 1996, 118, 429-436.	13.7	9
61	Analysis of the variables that modify the robustness of Ti-SiO2 catalysts for alkene epoxidation: Role of silylation, deactivation and potential solutions. Molecular Catalysis, 2018, 459, 55-60.	2.0	9
62	Critical Role of Oxygen in Silver-Catalyzed Glaserâ€“Hay Coupling on Ag(100) under Vacuum and in Solution on Ag Particles. ACS Catalysis, 2017, 7, 3113-3120.	11.2	8
63	Improving the activity of gold nanoparticles for the water-gas shift reaction using TiO₂â€“Y₂O₃: an example of catalyst design. Physical Chemistry Chemical Physics, 2018, 20, 22076-22083.	2.8	8
64	Understanding the Photocatalytic Properties of Pt/CeO_x/TiO₂: Structural Effects on Electronic and Optical Properties. ChemPhysChem, 2019, 20, 1624-1629.	2.1	8
65	High-Throughput Screening of the Thermoelastic Properties of Ultrahigh-Temperature Ceramics. ACS Applied Materials & Interfaces, 2021, 13, 29843-29857.	8.0	8
66	Molecular structure and vibrational analysis of distannane from ab initio second-order perturbation calculations: a theoretical approach to the tin-X bond (X = C, Si, Ge, Sn). The Journal of Physical Chemistry, 1989, 93, 7328-7333.	2.9	7
67	The vacuum ultraviolet spectrum of [Mn2(CO)10]. Journal of Organometallic Chemistry, 1992, 434, 235-240.	1.8	7
68	Theoretical investigations of NMR chemical shieldings on the AlPON catalyst system. Journal of Non-Crystalline Solids, 2000, 263-264, 189-194.	3.1	7
69	Ab initio calculations of molecular and electronic structure of disilane. II. Photoelectron and vacuum UV electronic spectra. Chemical Physics, 1991, 149, 333-339.	1.9	6
70	Structure and Dynamics of Methyl-substituted Beryllocene: [Be(C5Me5)2]. Theoretical Chemistry Accounts, 2006, 116, 480-485.	1.4	6
71	Nanosized CoO Films on the Î±-Al₂O₃ (0001) Surface: A Density Functional Study. Journal of Physical Chemistry C, 2013, 117, 22714-22722.	3.1	6
72	Ceria(100) Nanotubes with Negative Strain Energy: A First-Principles Prediction. Journal of Physical Chemistry Letters, 2012, 3, 2092-2096.	4.6	5

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73	Analysis of the origin of lateral interactions in the adsorption of small organic molecules on oxide surfaces. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	5
74	Connecting experimental synthetic variables with the microstructure and electronic properties of doped ferroelectric perovskites for solar cell applications using high-throughput frameworks. Acta Materialia, 2021, 204, 116466.	7.9	4
75	Vibrational spectra of stannane: Harmonic force field, Raman and IR intensities from ab initio correlated wavefunctions. Chemical Physics, 1989, 130, 451-456.	1.9	3
76	A theoretical approach to the molecular structure of vinylstannane and some structural isomers. Journal of Organometallic Chemistry, 1995, 486, 45-50.	1.8	3
77	Structural and electronic properties of lead sulfide quantum dots from screened hybrid density functional calculations including spinâ€“orbit coupling effects. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	3
78	An ab initio CASSCF study of the hydroxyl + nitrosyl chloride reaction. The Journal of Physical Chemistry, 1992, 96, 2115-2118.	2.9	2
79	An ab initio study of the CH2O adsorption on the MgO (100) surface. Effects of replacing the active Mg2+ ion by different metallic cations. Computational and Theoretical Chemistry, 1997, 390, 177-181.	1.5	2
80	Catalytic activity of PtCu intermetallic compound for CO oxidation: A theoretical insight. Catalysis Today, 2022, 383, 339-344.	4.4	2
81	Optoelectronic properties of Ag2S/graphene and FeS2/graphene nanostructures and interfaces: A density functional study including dispersion forces. Journal of Materials Research, 2022, 37, 1047-1058.	2.6	2
82	The Short-Range Structure of Aluminophosphate Oxynitride Catalysts. An ab Initio and Experimental Study. Journal of Physical Chemistry B, 1999, 103, 10850-10857.	2.6	1
83	Structure of a mononuclear Rhenium catalyst supported on MgO: An ab initio study. Journal of Molecular Catalysis A, 1997, 119, 195-200.	4.8	0
84	Analysis of the origin of lateral interactions in the adsorption of small organic molecules on oxide surfaces. Highlights in Theoretical Chemistry, 2014, , 177-183.	0.0	0