

Andrea Vittadini

List of Publications by Year in descending order

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148
papers

8,387
citations

101384

36
h-index

46693

89
g-index

160
all docs

160
docs citations

160
times ranked

9782
citing authors

#	ARTICLE	IF	CITATIONS
1	Structure and energetics of stoichiometric TiO ₂ anatase surfaces. <i>Physical Review B</i> , 2001, 63, .	1.1	1,258
2	Structure and Energetics of Water Adsorbed at TiO ₂ Anatase (101) and (001) Surfaces. <i>Physical Review Letters</i> , 1998, 81, 2954-2957.	2.9	883
3	Role and effective treatment of dispersive forces in materials: Polyethylene and graphite crystals as test cases. <i>Journal of Computational Chemistry</i> , 2009, 30, 934-939.	1.5	653
4	A Series of Isorecticular, Highly Stable, Porous Zirconium Oxide Based Metal-Organic Frameworks. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 9267-9271.	7.2	407
5	Formic Acid Adsorption on Dry and Hydrated TiO ₂ Anatase (101) Surfaces by DFT Calculations. <i>Journal of Physical Chemistry B</i> , 2000, 104, 1300-1306.	1.2	402
6	Theoretical Studies on Anatase and Less Common TiO ₂ Phases: Bulk, Surfaces, and Nanomaterials. <i>Chemical Reviews</i> , 2014, 114, 9708-9753.	23.0	367
7	Photoemission and STM study of the electronic structure of Nb-doped TiO ₂ . <i>Physical Review B</i> , 2000, 61, 13445-13457.	1.1	264
8	Chemistry of and on TiO ₂ -anatase surfaces by DFT calculations: a partial review. <i>Theoretical Chemistry Accounts</i> , 2007, 117, 663-671.	0.5	237
9	Density Functional Theory Study of Formic Acid Adsorption on Anatase TiO ₂ (001): Geometries, Energetics, and Effects of Coverage, Hydration, and Reconstruction. <i>Journal of Physical Chemistry B</i> , 2006, 110, 2804-2811.	1.2	219
10	Small gold clusters on stoichiometric and defected TiO ₂ anatase (101) and their interaction with CO: A density functional study. <i>Journal of Chemical Physics</i> , 2002, 117, 353-361.	1.2	133
11	Tuning the catalytic activity of Ag(110)-supported Fe phthalocyanine in the oxygen reduction reaction. <i>Nature Materials</i> , 2012, 11, 970-977.	13.3	131
12	Hexakis(acetato)oxotetrazinc, a well-tailored molecular model of zinc oxide. An experimental and theoretical investigation of the electronic structure of Zn ₄ O(acetate) ₆ and ZnO by means of UV and x-ray photoelectron spectroscopies and first principle local density molecular cluster calculations. <i>Inorganic Chemistry</i> , 1992, 31, 1558-1565.	1.9	130
13	Chemistry of the Strong Electrophilic Metal Fragment [99Tc(N)(PXP)] ₂ ⁺ (PXP = Diphosphine Ligand). A Novel Tool for the Selective Labeling of Small Molecules. <i>Journal of the American Chemical Society</i> , 2002, 124, 11468-11479.	6.6	95
14	Molecular Chemisorption on TiO ₂ (110): A Local Point of View. <i>Journal of Physical Chemistry B</i> , 1998, 102, 10745-10752.	1.2	91
15	The adsorption of small molecules on the TiO ₂ anatase (101) surface by first-principles molecular dynamics. <i>Surface Science</i> , 1998, 402-404, 219-222.	0.8	88
16	Bottom-Up Assembly of Single-Domain Titania Nanosheets on (111)-Pt(110). <i>Physical Review Letters</i> , 2006, 97, 156101.	2.9	79
17	Ab initio modeling of TiO ₂ nanosheets. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 551-556.	0.5	76
18	Density functional study of H ₂ desorption from monohydride and dihydride Si(100) surfaces. <i>Chemical Physics Letters</i> , 1995, 235, 334-340.	1.2	72

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19	Binding Sites, Migration Paths, and Barriers for Hydrogen on Si(111)-(7 \times 7). <i>Physical Review Letters</i> , 1995, 75, 4756-4759.	2.9	72
20	Structure and Stability of TiO ₂ -B Surfaces: A Density Functional Study. <i>Journal of Physical Chemistry C</i> , 2009, 113, 18973-18977.	1.5	67
21	Periodic Density Functional Theory Studies of Vanadia-Titania Catalysts: Structure and Stability of the Oxidized Monolayer. <i>Journal of Physical Chemistry B</i> , 2004, 108, 7337-7343.	1.2	57
22	Spin-Orbit Relativistic Time-Dependent Density Functional Calculations of the Metal and Ligand Pre-Edge XAS Intensities of Organotitanium Complexes: TiCl ₄ , Ti(<i>i</i> -5-C ₅ H ₅)Cl ₃ , and Ti(<i>i</i> -5-C ₅ H ₅) ₂ Cl ₂ . <i>Journal of Physical Chemistry A</i> , 2007, 111, 5270-5279.	1.1	54
23	Experimental and Theoretical Study of the Interaction of CO ₂ with γ -Al ₂ O ₃ . <i>Inorganic Chemistry</i> , 2003, 42, 436-445.	1.9	52
24	Pairing of hydrogen atoms on the Si(100)-(2 \times 1) surface: The role of interactions among dimers. <i>Physical Review B</i> , 1994, 49, 11191-11195.	1.1	50
25	An LCAO-LDF study of the chemisorption of H ₂ O and H ₂ S on ZnO(0001) and ZnO(101 $\bar{1}$,0). <i>Surface Science</i> , 1997, 377-379, 587-591.	0.8	50
26	Energetics of atomic hydrogen diffusion on Si(100). <i>Surface Science</i> , 1993, 289, L625-L630.	0.8	48
27	The preparation of substitution-inert ⁹⁹ Tc metal-fragments: Promising candidates for the design of new ^{99m} Tc radiopharmaceuticals. <i>Coordination Chemistry Reviews</i> , 2006, 250, 2034-2045.	9.5	47
28	First Principles Study of Hydrated/Hydroxylated TiO ₂ Nanolayers: From Isolated Sheets to Stacks and Tubes. <i>ACS Nano</i> , 2009, 3, 317-324.	7.3	47
29	First Principles Studies of Vanadia-Titania Monolayer Catalysts: Mechanisms of NO Selective Reduction. <i>Journal of Physical Chemistry B</i> , 2005, 109, 1652-1655.	1.2	46
30	A theoretical study of the H ₂ O and H ₂ S chemisorption on Cu ₂ O(111). <i>Applied Surface Science</i> , 1999, 142, 164-168.	3.1	44
31	Magnetic Properties and Vapochromic Reversible Guest-Induced Transformation in a Bispyrazolato Copper(II) Polymer: an Experimental and Dispersion-Corrected Density Functional Theory Study. <i>Inorganic Chemistry</i> , 2009, 48, 4044-4051.	1.9	44
32	Coverage-Dependent Architectures of Iron Phthalocyanine on Ag(110): a Comprehensive STM/DFT Study. <i>Journal of Physical Chemistry C</i> , 2010, 114, 2144-2153.	1.5	42
33	The structure of a stoichiometric TiO ₂ nanophase on Pt(1 1 1). <i>Surface Science</i> , 2007, 601, 3488-3496.	0.8	40
34	Atomic Structure and Special Reactivity Toward Methanol Oxidation of Vanadia Nanoclusters on TiO ₂ (110). <i>Journal of the American Chemical Society</i> , 2013, 135, 17331-17338.	6.6	39
35	An Experimental and Theoretical Study of the Electronic Structure of Zinc Thiophenolate-Capped Clusters. <i>Inorganic Chemistry</i> , 1997, 36, 4707-4716.	1.9	37
36	First-Principles Studies of Vanadia-Titania Catalysts: Beyond the Monolayer. <i>Journal of Physical Chemistry B</i> , 2005, 109, 21766-21771.	1.2	35

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37	Stereoselective Photopolymerization of Tetraphenylporphyrin Derivatives on Ag(110) at the Submonolayer Level. <i>Chemistry - A European Journal</i> , 2014, 20, 14296-14304.	1.7	35
38	Coordination chemistry of CO and NH ₃ on ZnO(0001): a molecular cluster study of the CO and NH ₃ bonding interaction with a d ¹⁰ ion. <i>Surface Science</i> , 1994, 303, 125-138.	0.8	34
39	Density functional studies of molecular chemisorption on TiO ₂ (110). <i>Applied Surface Science</i> , 1999, 142, 196-199.	3.1	34
40	Surface carboxylate species on Cu(100) studied by angle-scanned photoelectron diffraction and LCAO-LDF calculations. <i>Surface Science</i> , 1994, 315, 309-322.	0.8	32
41	A theoretical study of the CO and NO chemisorption on Cu ₂ O(111). <i>Surface Science</i> , 1997, 387, L1079-L1084.	0.8	32
42	A comparative study of CO and NO chemisorption on Cu ₂ O(111) and Ag ₂ O(111) non-polar surfaces. <i>Chemical Physics Letters</i> , 1997, 280, 53-58.	1.2	32
43	In-Depth Study of ZnS Nanoparticle Surface Properties with a Combined Experimental and Theoretical Approach. <i>Journal of Physical Chemistry C</i> , 2020, 124, 7777-7789.	1.5	32
44	A Comparative Study of CO Chemisorption on Al ₂ O ₃ and Ti ₂ O ₃ Nonpolar Surfaces. <i>Journal of Physical Chemistry B</i> , 2002, 106, 795-802.	1.2	31
45	Stability of TiO ₂ Polymorphs: Exploring the Extreme Frontier of the Nanoscale. <i>ChemPhysChem</i> , 2010, 11, 1550-1557.	1.0	31
46	Binding and diffusion of hydroxyl radicals on Si(100): A first-principles study. <i>Physical Review B</i> , 1995, 52, 5885-5889.	1.1	30
47	Electrochemical Behavior of TiO ₂ C _x as Catalyst Support for Direct Ethanol Fuel Cells at Intermediate Temperature: From Planar Systems to Powders. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 716-725.	4.0	30
48	Theoretical study of SiH ₃ -defect stability and formation on the H-saturated Si(100) 1 \times 1 surface. <i>Physical Review B</i> , 1992, 46, 4348-4351.	1.1	29
49	Carbothermal Transformation of TiO ₂ into TiO _x C _y in UHV: Tracking Intrinsic Chemical Stabilities. <i>Journal of Physical Chemistry C</i> , 2014, 118, 22601-22610.	1.5	29
50	Hydrogen capture by porphyrins at the TiO ₂ (110) surface. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 30119-30124.	1.3	29
51	Energetics of CO oxidation on lanthanide-free perovskite systems: the case of Co-doped SrTiO ₃ . <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 33282-33286.	1.3	29
52	SO ₂ on TiO ₂ (110) and Ti ₂ O ₃ (101 $\bar{1}$,2) Nonpolar Surfaces: A DFT Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 12596-12602.	1.2	28
53	Catalytic Mechanisms of NO Reduction in a CO/NO Atmosphere at Co- and Cu-Doped SrTiO ₃ (100) Surfaces. <i>Journal of Physical Chemistry C</i> , 2018, 122, 449-454.	1.5	28
54	Organometallic Chemistry of Ph ₃ PCCO. Synthesis, Characterization, X-ray Structure Determination, and Density Functional Study of the First Stable Bis- η -1-ketenyl Complex, trans-[PtCl ₂ { η -1-C(PPh ₃)CO} ₂]. <i>Organometallics</i> , 2000, 19, 1373-1383.	1.1	27

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55	Co- and Cu-Doped Titanates: Toward a New Generation of Catalytic Converters. <i>Catalysis Letters</i> , 2014, 144, 1466-1471.	1.4	27
56	Theoretical Investigation of the Chemisorption of H ₂ and CO on the ZnO(101̄,0) Surface. <i>Inorganic Chemistry</i> , 1998, 37, 5482-5490.	1.9	26
57	Magnesium-like phases in epitaxial anatase TiO ₂ thin films. <i>Physical Review B</i> , 2012, 86, .	1.1	26
58	On-Surface Synthesis of a Pure and Long-Range-Ordered Titanium(IV)-Porphyrin Contact Layer on Titanium Dioxide. <i>Journal of Physical Chemistry C</i> , 2017, 121, 13738-13746.	1.5	26
59	Functionalisation of Colloidal Transition Metal Sulphides Nanocrystals: A Fascinating and Challenging Playground for the Chemist. <i>Crystals</i> , 2017, 7, 110.	1.0	26
60	Mobility of Au on TiO _x Substrates with Different Stoichiometry and Defectivity. <i>Journal of Physical Chemistry C</i> , 2008, 112, 3187-3190.	1.5	25
61	Adsorption of small molecules at the cobalt-doped SrTiO ₃ (001) surface: A first-principles investigation. <i>Surface Science</i> , 2015, 633, 68-76.	0.8	25
62	Theoretical Study of the Chemisorption of CO on Al ₂ O ₃ (0001). <i>Inorganic Chemistry</i> , 2000, 39, 5232-5237.	1.9	24
63	Tetraphenylporphyrin electronic properties: a combined theoretical and experimental study of thin films deposited by SuMBD. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 871-880.	1.3	24
64	Electronic structure of SrTi _{1-x} MxO ₃ (M=Co, Ni, Cu) perovskite-type doped-titanate crystals by DFT and DFT+U calculations. <i>Chemical Physics Letters</i> , 2013, 588, 102-108.	1.2	24
65	A LCAO-LDF study of formate chemisorption on Cu(100). <i>Surface Science</i> , 1994, 307-309, 95-100.	0.8	23
66	An experimental and theoretical study of the interaction of CH ₃ OH and CH ₃ SH with ZnO. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1996, 92, 3247.	1.7	23
67	A comparative study of the NH ₃ chemisorption on ZnO(101̄,0) and Cu ₂ O(111) non-polar surfaces. <i>Chemical Physics Letters</i> , 1999, 300, 403-408.	1.2	23
68	2D vs. 3D titanium dioxide: Role of dispersion interactions. <i>Chemical Physics Letters</i> , 2011, 516, 72-75.	1.2	23
69	Electronic properties of tetrakis(pentafluorophenyl)porphyrin. <i>New Journal of Chemistry</i> , 2013, 37, 1036.	1.4	23
70	Adsorption of CO and formation of carbonates at steps of pure and Co-doped SrTiO ₃ surfaces by DFT calculations. <i>Applied Surface Science</i> , 2016, 364, 522-527.	3.1	21
71	Coordination chemistry of CO and NH ₃ on CuCl(111): an experimental and theoretical study of the CO and NH ₃ bonding to a d ₁₀ ion. <i>Surface Science</i> , 1994, 317, 422-436.	0.8	20
72	Electronic structure of Nb impurities in and on TiO ₂ . <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 3793-3799.	1.3	20

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73	Ultrathin TiO ₂ Films on (1 $\bar{1}$ –2)-Pt(110): a LEED, Photoemission, STM, and Theoretical Investigation. <i>Journal of Physical Chemistry C</i> , 2008, 112, 20038-20049.	1.5	20
74	Electronic structure of CuTPP and CuTPP(F) complexes: a combined experimental and theoretical study II. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 24890-24904.	1.3	19
75	H ₂ adsorption/desorption at Si(111)-(7 \bar{A} –7): a density functional study. <i>Surface Science</i> , 1997, 383, L779-L784.	0.8	18
76	Strong Bonding of Single C ₆₀ Molecules to (1 $\bar{1}$ –2)-Pt(110): an STM/DFT Investigation. <i>Journal of Physical Chemistry C</i> , 2007, 111, 9365-9373.	1.5	17
77	Temperature-Dependent Self-Assemblies of C ₆₀ on (1 $\bar{1}$ –2)-Pt(110): A STM/DFT Investigation. <i>Journal of Physical Chemistry C</i> , 2008, 112, 378-390.	1.5	17
78	Hydroxylation of TiO ₂ -B: insights from density functional calculations. <i>Journal of Materials Chemistry</i> , 2010, 20, 5871.	6.7	17
79	Theoretical modeling of the L _{2,3} -edge X-ray absorption spectra of Mn(acac) ₂ and Co(acac) ₂ complexes. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 2242-2249.	1.3	17
80	Combined UV-PES and theoretical study of binuclear M ₂ (CO) ₆ (C ₄ H ₄) complexes (M = Fe, Ru, Os). <i>Inorganic Chemistry</i> , 1987, 26, 2041-2046.	1.9	16
81	A LCAO-LDF study of CO and NH ₃ chemisorption on ZnO(0001). <i>Surface Science</i> , 1994, 307-309, 1182-1187.	0.8	16
82	A theoretical investigation of Brønsted acids chemisorption on ZnO(0001). <i>Surface Science</i> , 1995, 343, 115-132.	0.8	16
83	Experimental and Theoretical Investigation of the Molecular and Electronic Structure of [Zn ₄ ($\bar{1}$ / ₄ -S) ₂ As(CH ₃) ₂] ₆] and [Cd ₄ ($\bar{1}$ / ₄ -S) ₂ As(CH ₃) ₂] ₆]: A Two Possible Molecular Models of Extended Metal Chalcogenide Semiconductors. <i>Inorganic Chemistry</i> , 1999, 38, 1145-1152.		16
84	Defects in Oxygen-Depleted Titanate Nanostructures. <i>Langmuir</i> , 2012, 28, 7851-7858.	1.6	16
85	Electronic structures of CuTPP and CuTPP(F) complexes. A combined experimental and theoretical study I. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 18727-18738.	1.3	16
86	L _{2,3} -edges absorption spectra of a 2D complex system: a theoretical modelling. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 28110-28116.	1.3	16
87	A molecular cluster approach to the study of the bonding of CO and NH ₃ to a d ¹⁰ ion on ZnO(0001) and CuCl(111). <i>Inorganica Chimica Acta</i> , 1995, 235, 151-158.	1.2	15
88	A theoretical and experimental investigation of the electronic structure of alpha-Fe ₂ O ₃ thin films. <i>Journal of Physics Condensed Matter</i> , 1995, 7, L299-L305.	0.7	15
89	A theoretical investigation of the relaxation effects induced on the ZnO(10 $\bar{1}$,0) surface by the chemisorption of H ₂ and CO. <i>Applied Surface Science</i> , 1999, 142, 192-195.	3.1	15
90	Very high temperature tiling of tetraphenylporphyrin on rutile TiO ₂ (110). <i>Nanoscale</i> , 2017, 9, 11694-11704.	2.8	15

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91	Helium(He I and He II) photoelectron spectra of nickel(II), palladium(II) and platinum(II) diethyldithiocarbamate complexes. <i>Inorganic Chemistry</i> , 1984, 23, 702-706.	1.9	14
92	Mn(acac) ₂ and Mn(acac) ₃ complexes, a theoretical modeling of their L _{2,3} -edges X-ray absorption spectra. <i>Polyhedron</i> , 2017, 135, 216-223.	1.0	14
93	Zn ₄ O(O ₂ CNEt ₂) ₆ : a further molecular model of ZnO. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1993, 89, 4363.	1.7	13
94	Molecular, Electronic, and Crystal Structures of Self-Assembled Hydrothermally Synthesized Zn(II)-Mercaptonicotinate: A Combined Spectroscopic and Theoretical Approach. <i>Inorganic Chemistry</i> , 2010, 49, 4099-4108.	1.9	13
95	Tuning dispersion correction in DFT-D2 for metal-molecule interactions: A tailored reparameterization strategy for the adsorption of aromatic systems on Ag(111). <i>Chemical Physics Letters</i> , 2018, 693, 28-33.	1.2	13
96	UV-Photoelectron Spectra of [M(η^3 -C ₃ H ₅) ₂] (M = Ni, Pd, Pt) Revisited: A Quasi-Relativistic Density Functional Study. <i>Organometallics</i> , 2001, 20, 754-762.	1.1	12
97	On the Effects of Doping on the Catalytic Performance of (La,Sr)CoO ₃ . A DFT Study of CO Oxidation. <i>Catalysts</i> , 2019, 9, 312.	1.6	12
98	Synthesis and reactivity of dimethylindium derivatives: molecular and electronic structure of bis(η^4 -diethylamido)-tetramethyldi-indium(III). <i>Inorganica Chimica Acta</i> , 1990, 170, 95-101.	1.2	11
99	Oxygen Reduction Reaction at Single-Site Catalysts: A Combined Electrochemical Scanning Tunnelling Microscopy and DFT Investigation on Iron Octaethylporphyrin Chloride on HOPG**. <i>ChemElectroChem</i> , 2021, 8, 2825-2835.	1.7	11
100	Experimental and QM/MM investigation of the hydrated silica surface reactivity. <i>Chemical Physics Letters</i> , 2005, 405, 459-464.	1.2	10
101	Evolution of nanostructures of anatase TiO ₂ thin films grown on (001) LaAlO ₃ . <i>Journal of Nanoparticle Research</i> , 2013, 15, 1.	0.8	10
102	A LCAO-LDF study of Br ⁻ adsorbed acids chemisorption on ZnO(0001). <i>Surface Science</i> , 1996, 352-354, 341-345.	0.8	9
103	A theoretical study of the chemisorption of H ₂ O and H ₂ S on the Ti ₂ O ₃ (101 $\bar{1}$,2) non-polar surface. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 2461-2468.	1.3	9
104	Density Functional Theory Study of the Binding Capability of Tris(pyrazol-1-yl)methane toward Cu(I) and Ag(I) Cations. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6723-6731.	1.1	9
105	A theoretical investigation of the hyperfine properties of normal and anomalous muonium in elemental semiconductors: Diamond, silicon and germanium. <i>Chemical Physics</i> , 1991, 154, 385-393.	0.9	8
106	LCAO-LDA Study of the chemisorption of formate on Cu(110) and Ag(110) surfaces. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1998, 94, 797-804.	1.7	8
107	An experimental and theoretical study of the electronic and molecular structure of [Zn ₄ (η^4 -S) ₂ (η^4 -S ₂ P(OC ₂ H ₅) ₂) ₆]: the first molecular model of ZnS. <i>Journal of Organometallic Chemistry</i> , 2000, 593-594, 307-314.	0.8	8
108	A Comparative Theoretical Investigation of Three Sodalite Systems: Cd ₄ S(AlO ₂) ₆ , Zn ₄ O(BO ₂) ₆ , and Zn ₄ S(BO ₂) ₆ . <i>Journal of Physical Chemistry B</i> , 2002, 106, 2569-2573.	1.2	8

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109	A theoretical study of the interaction of CO ₂ with hydroxylated γ -alumina. <i>Surface Science</i> , 2004, 566-568, 890-894.	0.8	8
110	A DV-XPS theoretical investigation of the electronic structure of some tris(cyclopentadienyl) complexes of U(IV). <i>Inorganica Chimica Acta</i> , 1986, 121, L23-L25.	1.2	7
111	Ruthenium carbonyl 1,4-diaza-1,3-butadiene (R-DAB) complexes. A theoretical and experimental investigation of the electronic structure of Ru ₂ (CO) ₄ (R-DAB)(μ -CO) and Ru ₂ (CO) ₄ (R-DAB)(μ -HC.tplbond.CH). <i>Journal of the American Chemical Society</i> , 1988, 110, 1775-1781.	6.6	7
112	Tris(pyrazol-1-yl)borate and tris(pyrazol-1-yl)methane: A DFT study of their different binding capability toward Ag(I) and Cu(I) cations. <i>Inorganica Chimica Acta</i> , 2009, 362, 4358-4364.	1.2	7
113	Synthesis and Development of Four Way Catalysts Starting from Critical Raw Material Free Perovskites: Influence of Doping and Synthesis Conditions. <i>Topics in Catalysis</i> , 2019, 62, 237-243.	1.3	7
114	Digging Ti interstitials at the r-TiO ₂ (1 1 0) surface: Mechanism of porphyrin Ti sequestration by iminic N nucleophilic attack. <i>Applied Surface Science</i> , 2021, 564, 150403.	3.1	7
115	Electronic structure of bimetallic "flyover-bridge" derivatives. UV-PES and ab initio study of [cyclic] 511-514.	1.9	6
116	Structure of (Z)-N-benzoyl- β , β -dehydroleucine. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 1986, 42, 1178-1181.	0.4	6
117	Experimental and theoretical investigation of the electronic structure of two isoelectronic binuclear clusters. UV-PES and DV-XPS study of ruthenium ethanediyldiamido carbonyl, Ru ₂ (CO) ₆ [μ , μ '-N(R)CH ₂ CH ₂ N(R)], and iron ruthenium ethanediyldiamido carbonyl, FeRu(CO) ₆ [μ , μ '-N(R)CH ₂ CH ₂ N(R)]. <i>Inorganic Chemistry</i> , 1991, 30, 1906-1911.	1.9	6
118	A comparative study of the CO chemisorption on Ti ₂ O ₃ (102) and V ₂ O ₃ (102) non-polar surfaces. <i>Surface Science</i> , 2004, 566-568, 451-456.	0.8	6
119	On the formation of [H ₃ Ci ξ ξ Si ξ ξ Si ξ ξ CH ₃] ⁺ ions from the bis(dimethylthio)mercury molecular ion. <i>Rapid Communications in Mass Spectrometry</i> , 2006, 20, 3154-3158.	0.7	6
120	Carbonyl copper(κ) complexes with hydrotris(1,2,4-triazolyl)borate, hydrotris(pyrazolyl)borate, and tris(pyrazolyl)methane ligands: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 94-96.	1.3	6
121	Vapochromic properties versus metal ion coordination of β -bispyrazolato copper(κ) coordination polymers: a first-principles investigation. <i>CrystEngComm</i> , 2015, 17, 407-411.	1.3	6
122	Small Copper Clusters Supported on SrTiO ₃ : An Experimental and Theoretical Study. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 3829-3834.	1.0	6
123	Adsorption and reactivity of CO at a stepped SrTiO ₃ (1 $\hat{0}$ $\hat{0}$) surface in the presence of Cu impurities. <i>Applied Surface Science</i> , 2020, 521, 146450.	3.1	6
124	A Theoretical Study of the Occupied and Unoccupied Electronic Structure of High- and Intermediate-Spin Transition Metal Phthalocyaninato (Pc) Complexes: VPC, CrPc, MnPc, and FePc. <i>Nanomaterials</i> , 2021, 11, 54.	1.9	6
125	Electronic structure of Ru ₃ (CO) ₆ (CH ₃ Ci \rightarrow CHCH = NC ₃ H ₇ -i) ₂ as indicated by UV-photoelectron spectroscopy and DV-XPS quantum mechanical calculations. <i>Journal of Organometallic Chemistry</i> , 1990, 396, 73-81.	0.8	5
126	Water-Soluble [Tc(N)(PNP)] Moiety for Room-Temperature ^{99m} Tc Labeling of Sensitive Target Vectors. <i>Molecular Pharmaceutics</i> , 2022, 19, 876-894.	2.3	5

#	ARTICLE	IF	CITATIONS
127	Binding Sites, Migration Paths, and Barriers for Hydrogen on Si(111)-(7 Å ⁻¹ × 7). <i>Physical Review Letters</i> , 1996, 76, 3662-3662.	2.9	4
128	A Theoretical Study of Amine Bonding in Titanium Alkoxide Adducts. <i>Monatshefte für Chemie</i> , 2007, 138, 1217-1223.	0.9	4
129	On surface chemical reactions of free-base and titanyl porphyrins with r-TiO ₂ (110): a unified picture. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 12719-12744.	1.3	4
130	An accurate DV XPS investigation of the electronic structure of bis (2,4-pentanedionato) palladium(II). <i>Chemical Physics Letters</i> , 1987, 141, 193-197.	1.2	3
131	Molecular cluster model of the electronic structure of substitutional impurities in gallium arsenide. <i>Chemistry of Materials</i> , 1989, 1, 587-591.	3.2	3
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133	A DFT-D2 study of formic acid adsorption at smectite edges based on pyrophyllite models. <i>Chemical Physics Letters</i> , 2019, 733, 136687.	1.2	3
134	A molecular cluster approach to the electronic structure of anomalous muonium in diamond. <i>Chemical Physics</i> , 1990, 148, 183-192.	0.9	2
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141	DFT modelling of the CO-NO redox reaction at Cu-doped SrTiO ₃ (100) stepped surface: CO oxidation at lattice O ions. <i>Inorganica Chimica Acta</i> , 2020, 511, 119810.	1.2	2
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143	Energetics of atomic hydrogen diffusion on Si(100). <i>Surface Science Letters</i> , 1993, 289, L625-L630.	0.1	1
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145	Conformational and electronic effects in dehydroaminoacid derivatives. <i>Journal of Molecular Structure</i> , 1986, 141, 415-418.	1.8	0
146	Erratum to "An experiment and theoretical study of the electronic and molecular structure of $[Zn_4(\mu_4-S)(\mu_3-S)_2P(OC_2H_5)_2]_6$ ": the first molecular model of ZnS. <i>Journal of Organometallic Chemistry</i> , 2000, 601, 343.	0.8	0
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148	$[Zn_{10}(\mu_4-S)(\mu_3-S)_6(Py)_9(SO_4)_3]$ as a molecular model of ZnS surfaces: an experimental and theoretical study. <i>Highlights in Theoretical Chemistry</i> , 2013, , 161-168.	0.0	0