Andrea Vittadini

List of Publications by Year
in descending order

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148	8,387	101384	46693
papers	citations	36 h-index	89 g-index

160	160	160	9782
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Water-Soluble [Tc(N)(PNP)] Moiety for Room-Temperature ^{99m}Tc Labeling of Sensitive Target Vectors. Molecular Pharmaceutics, 2022, 19, 876-894.	2.3	5
2	On surface chemical reactions of free-base and titanyl porphyrins with r-TiO₂(110): a unified picture. Physical Chemistry Chemical Physics, 2022, 24, 12719-12744.	1.3	4
3	Oxygen Reduction Reaction at Singleâ€Site Catalysts: A Combined Electrochemical Scanning Tunnelling Microscopy and DFT Investigation on Iron Octaethylporphyrin Chloride on HOPG**. ChemElectroChem, 2021, 8, 2825-2835.	1.7	11
4	Digging Ti interstitials at the r-TiO2(1 1 0) surface: Mechanism of porphyrin Ti sequestration by iminic N nucleophilic attack. Applied Surface Science, 2021, 564, 150403.	3.1	7
5	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. Nanomaterials, 2021, 11, 54.	1.9	6
6	Adsorption and reactivity of CO at a stepped SrTiO3(1Â0Â0) surface in the presence of Cu impurities. Applied Surface Science, 2020, 521, 146450.	3.1	6
7	DFT modelling of the CO-NO redox reaction at Cu-doped SrTiO3(1Â0Â0) stepped surface: CO oxidation at lattice O ions. Inorganica Chimica Acta, 2020, 511, 119810.	1.2	2
8	DFT modelling of the NO reduction process at the Cu-doped SrTiO3(1Â0Â0) stepped surface. Inorganica Chimica Acta, 2020, 511, 119813.	1.2	2
9	In-Depth Study of ZnS Nanoparticle Surface Properties with a Combined Experimental and Theoretical Approach. Journal of Physical Chemistry C, 2020, 124, 7777-7789.	1.5	32
10	A DFT-D2 study of formic acid adsorption at smectite edges based on pyrophyllite models. Chemical Physics Letters, 2019, 733, 136687.	1.2	3
11	On the Effects of Doping on the Catalytic Performance of (La,Sr)CoO3. A DFT Study of CO Oxidation. Catalysts, 2019, 9, 312.	1.6	12
12	Synthesis and Development of Four Way Catalysts Starting from Critical Raw Material Free Perovskites: Influence of Doping and Synthesis Conditions. Topics in Catalysis, 2019, 62, 237-243.	1.3	7
13	Catalytic Mechanisms of NO Reduction in a COâ€“NO Atmosphere at Co- and Cu-Doped SrTiO₃(100) Surfaces. Journal of Physical Chemistry C, 2018, 122, 449-454.	1.5	28
14	Tuning dispersion correction in DFT-D2 for metal-molecule interactions: A tailored reparameterization strategy for the adsorption of aromatic systems on Ag(1â€¯1â€¯1). Chemical Physics Letters, 2018, 693, 28-33.	1.2	13
15	Small Copper Clusters Supported on SrTiO₃: An Experimental and Theoretical Study. European Journal of Inorganic Chemistry, 2018, 2018, 3829-3834.	1.0	6
16	On-Surface Synthesis of a Pure and Long-Range-Ordered Titanium(IV)-Porphyrin Contact Layer on Titanium Dioxide. Journal of Physical Chemistry C, 2017, 121, 13738-13746.	1.5	26
17	Mn(acac) 2 and Mn(acac) 3 complexes, a theoretical modeling of their L 2,3 -edges X-ray absorption spectra. Polyhedron, 2017, 135, 216-223.	1.0	14
18	Very high temperature tiling of tetraphenylporphyrin on rutile TiO₂(110). Nanoscale, 2017, 9, 11694-11704.	2.8	15

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19	Interaction products of cytotoxic Cu(I) complexes with different solvent mixtures: an electrospray ionization mass spectrometry and density functional theory study. Rapid Communications in Mass Spectrometry, 2017, 31, 179-192.	0.7	2
20	Functionalisation of Colloidal Transition Metal Sulphides Nanocrystals: A Fascinating and Challenging Playground for the Chemist. Crystals, 2017, 7, 110.	1.0	26
21	Electronic structures of CuTPP and CuTPP(F) complexes. A combined experimental and theoretical study I. Physical Chemistry Chemical Physics, 2016, 18, 18727-18738.	1.3	16
22	Electronic structure of CuTPP and CuTPP(F) complexes: a combined experimental and theoretical study II. Physical Chemistry Chemical Physics, 2016, 18, 24890-24904.	1.3	19
23	L_{2,3}-edges absorption spectra of a 2D complex system: a theoretical modelling. Physical Chemistry Chemical Physics, 2016, 18, 28110-28116.	1.3	16
24	Energetics of CO oxidation on lanthanide-free perovskite systems: the case of Co-doped SrTiO₃. Physical Chemistry Chemical Physics, 2016, 18, 33282-33286.	1.3	29
25	Adsorption of CO and formation of carbonates at steps of pure and Co-doped SrTiO3 surfaces by DFT calculations. Applied Surface Science, 2016, 364, 522-527.	3.1	21
26	Theoretical modeling of the L_{2,3}-edge X-ray absorption spectra of Mn(acac)₂and Co(acac)₂complexes. Physical Chemistry Chemical Physics, 2016, 18, 2242-2249.	1.3	17
27	Electrochemical Behavior of TiO_xC_y as Catalyst Support for Direct Ethanol Fuel Cells at Intermediate Temperature: From Planar Systems to Powders. ACS Applied Materials & Interfaces, 2016, 8, 716-725.	4.0	30
28	Hydrogen capture by porphyrins at the TiO₂(110) surface. Physical Chemistry Chemical Physics, 2015, 17, 30119-30124.	1.3	29
29	Adsorption of small molecules at the cobalt-doped SrTiO3(001) surface: A first-principles investigation. Surface Science, 2015, 633, 68-76.	0.8	25
30	Vapochromic properties versus metal ion coordination of Î²-bispyrazolatoâ€“copper(<scp>ii</scp>) coordination polymers: a first-principles investigation. CrystEngComm, 2015, 17, 407-411.	1.3	6
31	Co- and Cu-Doped Titanates: Toward a New Generation of Catalytic Converters. Catalysis Letters, 2014, 144, 1466-1471.	1.4	27
32	Carbothermal Transformation of TiO₂ into TiO_xC_y in UHV: Tracking Intrinsic Chemical Stabilities. Journal of Physical Chemistry C, 2014, 118, 22601-22610.	1.5	29
33	Theoretical Studies on Anatase and Less Common TiO₂ Phases: Bulk, Surfaces, and Nanomaterials. Chemical Reviews, 2014, 114, 9708-9753.	23.0	367
34	Stereoselective Photopolymerization of Tetraphenylporphyrin Derivatives on Ag(110) at the Subâ€Monolayer Level. Chemistry - A European Journal, 2014, 20, 14296-14304.	1.7	35
35	Evolution of nanostructures of anatase TiO2 thin films grown on (001) LaAlO3. Journal of Nanoparticle Research, 2013, 15, 1.	0.8	10
36	Electronic structure of SrTi1â^'xMxO3â^'Î´ (M=Co, Ni, Cu) perovskite-type doped-titanate crystals by DFT and DFT+U calculations. Chemical Physics Letters, 2013, 588, 102-108.	1.2	24

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37	Atomic Structure and Special Reactivity Toward Methanol Oxidation of Vanadia Nanoclusters on TiO₂(110). Journal of the American Chemical Society, 2013, 135, 17331-17338.	6.6	39
38	Electronic properties of tetrakis(pentafluorophenyl)porphyrin. New Journal of Chemistry, 2013, 37, 1036.	1.4	23
39	[Zn10(Î¼4-S)(Î¼3-S)6(Py)9(SO4)3] as a molecular model of ZnS surfaces: an experimental and theoretical study. Highlights in Theoretical Chemistry, 2013, , 161-168.	0.0	0
40	MagnÃ©li-like phases in epitaxial anatase TiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>thin films. Physical Review B, 2012, 86, .	1.1	26
41	Defects in Oxygen-Depleted Titanate Nanostructures. Langmuir, 2012, 28, 7851-7858.	1.6	16
42	A Series of Isoreticular, Highly Stable, Porous Zirconium Oxide Based Metalâ€“Organic Frameworks. Angewandte Chemie - International Edition, 2012, 51, 9267-9271.	7.2	407
43	Tuning the catalytic activity of Ag(110)-supported Fe phthalocyanine in the oxygen reduction reaction. Nature Materials, 2012, 11, 970-977.	13.3	131
44	[Zn10(Âμ4-S)(Âμ3-S)6(Py)9(SO4)3] as a molecular model of ZnS surfaces: an experimental and theoretical study. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	0
45	2D vs. 3D titanium dioxide: Role of dispersion interactions. Chemical Physics Letters, 2011, 516, 72-75.	1.2	23
46	Stability of TiO₂ Polymorphs: Exploring the Extreme Frontier of the Nanoscale. ChemPhysChem, 2010, 11, 1550-1557.	1.0	31
47	Coverage-Dependent Architectures of Iron Phthalocyanine on Ag(110): a Comprehensive STM/DFT Study. Journal of Physical Chemistry C, 2010, 114, 2144-2153.	1.5	42
48	Molecular, Electronic, and Crystal Structures of Self-Assembled Hydrothermally Synthesized Zn(II)â^'Mercaptonicotinate: A Combined Spectroscopic and Theoretical Approach. Inorganic Chemistry, 2010, 49, 4099-4108.	1.9	13
49	Tetraphenylporphyrin electronic properties: a combined theoretical and experimental study of thin films deposited by SuMBD. Physical Chemistry Chemical Physics, 2010, 12, 871-880.	1.3	24
50	Hydroxylation of TiO2-B: insights from density functional calculations. Journal of Materials Chemistry, 2010, 20, 5871.	6.7	17
51	Role and effective treatment of dispersive forces in materials: Polyethylene and graphite crystals as test cases. Journal of Computational Chemistry, 2009, 30, 934-939.	1.5	653
52	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. Inorganica Chimica Acta, 2009, 362, 4358-4364.	1.2	7
53	First Principles Study of Hydrated/Hydroxylated TiO₂ Nanolayers: From Isolated Sheets to Stacks and Tubes. ACS Nano, 2009, 3, 317-324.	7.3	47
54	Carbonyl copper(<scp>i</scp>) complexes with hydrotris(1,2,4-triazolyl)borate, hydrotris(pyrazolyl)borate, and tris(pyrazolyl)methaneligands: a DFT study. Physical Chemistry Chemical Physics, 2009, 11, 94-96.	1.3	6

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55	Structure and Stability of TiO₂-B Surfaces: A Density Functional Study. Journal of Physical Chemistry C, 2009, 113, 18973-18977.	1.5	67
56	Magnetic Properties and Vapochromic Reversible Guest-Induced Transformation in a Bispyrazolato Copper(II) Polymer: an Experimental and Dispersion-Corrected Density Functional Theory Study. Inorganic Chemistry, 2009, 48, 4044-4051.	1.9	44
57	Ab initio modeling of TiO2 nanosheets. Theoretical Chemistry Accounts, 2008, 120, 551-556.	0.5	76
58	Ultrathin TiO₂ Films on (1Ã—2)-Pt(110): a LEED, Photoemission, STM, and Theoretical Investigation. Journal of Physical Chemistry C, 2008, 112, 20038-20049.	1.5	20
59	Mobility of Au on TiO_x Substrates with Different Stoichiometry and Defectivity. Journal of Physical Chemistry C, 2008, 112, 3187-3190.	1.5	25
60	Temperature-Dependent Self-Assemblies of C₆₀ on (1 Ã— 2)-Pt(110):â€‰ A STM/DFT Investigation. Journal of Physical Chemistry C, 2008, 112, 378-390.	1.5	17
61	Density Functional Theory Study of the Binding Capability of Tris(pyrazol-1-yl)methane toward Cu(I) and Ag(I) Cations. Journal of Physical Chemistry A, 2008, 112, 6723-6731.	1.1	9
62	Spinâ^'Orbit Relativistic Time-Dependent Density Functional Calculations of the Metal and Ligand Pre-Edge XAS Intensities of Organotitanium Complexes:â€‰ TiCl4, Ti(Î·5-C5H5)Cl3, and Ti(Î·5-C5H5)2Cl2. Journal of Physical Chemistry A, 2007, 111, 5270-5279.	1.1	54
63	Strong Bonding of Single C60Molecules to (1 Ã— 2)-Pt(110):â€‰ an STM/DFT Investigation. Journal of Physical Chemistry C, 2007, 111, 9365-9373.	1.5	17
64	Molecular photochromic systems: a theoretical and experimental investigation on zinc(II) dithizonate. Applied Organometallic Chemistry, 2007, 21, 246-254.	1.7	2
65	The structure of a stoichiometric TiO2 nanophase on Pt(1 1 1). Surface Science, 2007, 601, 3488-3496.	0.8	40
66	Chemistry of and on TiO2-anatase surfaces by DFT calculations: a partial review. Theoretical Chemistry Accounts, 2007, 117, 663-671.	0.5	237
67	A Theoretical Study of Amine Bonding in Titanium Alkoxide Adducts. Monatshefte FÃ¼r Chemie, 2007, 138, 1217-1223.	0.9	4
68	Density Functional Theory Study of Formic Acid Adsorption on Anatase TiO2(001):Â Geometries, Energetics, and Effects of Coverage, Hydration, and Reconstruction. Journal of Physical Chemistry B, 2006, 110, 2804-2811.	1.2	219
69	On the formation of [H3Cï£¿Sï£¿Sï£¿CH3]+. ions from the bis(dimethylthio)mercury molecular ion. Rapid Communications in Mass Spectrometry, 2006, 20, 3154-3158.	0.7	6
70	The preparation of substitution-inert 99Tc metal-fragments: Promising candidates for the design of new 99mTc radiopharmaceuticals. Coordination Chemistry Reviews, 2006, 250, 2034-2045.	9.5	47
71	Bottom-Up Assembly of Single-Domain Titania Nanosheets on(1Ã—2)â^'Pt(110). Physical Review Letters, 2006, 97, 156101.	2.9	79
72	Experimental and QM/MM investigation of the hydrated silica surface reactivity. Chemical Physics Letters, 2005, 405, 459-464.	1.2	10

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73	First Principles Studies of Vanadia?Titania Monolayer Catalysts: Mechanisms of NO Selective Reduction. ChemInform, 2005, 36, no.	0.1	1
74	First Principles Studies of Vanadiaâˆ'Titania Monolayer Catalysts:Â Mechanisms of NO Selective Reduction. Journal of Physical Chemistry B, 2005, 109, 1652-1655.	1.2	46
75	First-Principles Studies of Vanadiaâˆ'Titania Catalysts:Â Beyond the Monolayer. Journal of Physical Chemistry B, 2005, 109, 21766-21771.	1.2	35
76	SO2 on TiO2(110) and Ti2O3(101Ì„2) Nonpolar Surfaces:â€‰ A DFT Study. Journal of Physical Chemistry B, 2005, 109, 12596-12602.	1.2	28
77	A comparative study of the CO chemisorption on Ti2O3(102) and V2O3(102) non-polar surfaces. Surface Science, 2004, 566-568, 451-456.	0.8	6
78	A theoretical study of the interaction of CO2 with hydroxylated Î±-alumina. Surface Science, 2004, 566-568, 890-894.	0.8	8
79	Interstitial O3 in silica: a molecular cluster density functional study. Chemical Physics Letters, 2004, 392, 146-150.	1.2	2
80	Periodic Density Functional Theory Studies of Vanadiaâˆ'Titania Catalysts:Â Structure and Stability of the Oxidized Monolayer. Journal of Physical Chemistry B, 2004, 108, 7337-7343.	1.2	57
81	A theoretical study of the electronic structure of O2 interstitial impurities in silica. Computational and Theoretical Chemistry, 2003, 631, 111-116.	1.5	2
82	A theoretical study of the chemisorption of H2O and H2S on the Ti2O3(101Ì„2) non-polar surface. Physical Chemistry Chemical Physics, 2003, 5, 2461-2468.	1.3	9
83	Experimental and Theoretical Study of the Interaction of CO2with Î±-Al2O3. Inorganic Chemistry, 2003, 42, 436-445.	1.9	52
84	Chemistry of the Strong Electrophilic Metal Fragment [99Tc(N)(PXP)]2+ (PXP = Diphosphine Ligand). A Novel Tool for the Selective Labeling of Small Molecules. Journal of the American Chemical Society, 2002, 124, 11468-11479.	6.6	95
85	A Comparative Theoretical Investigation of Three Sodalite Systems:Â Cd4S(AlO2)6, Zn4O(BO2)6, and Zn4S(BO2)6. Journal of Physical Chemistry B, 2002, 106, 2569-2573.	1.2	8
86	A Comparative Study of CO Chemisorption on Al2O3and Ti2O3Nonpolar Surfaces. Journal of Physical Chemistry B, 2002, 106, 795-802.	1.2	31
87	Small gold clusters on stoichiometric and defected TiO2 anatase (101) and their interaction with CO: A density functional study. Journal of Chemical Physics, 2002, 117, 353-361.	1.2	133
88	Structure and energetics of stoichiometricTiO2anatase surfaces. Physical Review B, 2001, 63, .	1.1	1,258
89	UV-Photoelectron Spectra of [M(Î·3-C3H5)2] (M = Ni, Pd, Pt) Revisited:Â A Quasi-Relativistic Density Functional Study. Organometallics, 2001, 20, 754-762.	1.1	12
90	Erratum to â€œAn experiment and theoretical study of the electronic and molecular structure of [Zn4(Î¼4-S){Î¼-S2P(OC2H5)2}6]: the first molecular model of ZnSâ€• Journal of Organometallic Chemistry, 2000, 601, 343.	0.8	0

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91	An experimental and theoretical study of the electronic and molecular structure of [Zn4(?4-S){Î¼-S2P(OC2H5)2}6]: the first molecular model of ZnS. Journal of Organometallic Chemistry, 2000, 593-594, 307-314.	0.8	8
92	Formic Acid Adsorption on Dry and Hydrated TiO2 Anatase (101) Surfaces by DFT Calculations. Journal of Physical Chemistry B, 2000, 104, 1300-1306.	1.2	402
93	Photoemission and STM study of the electronic structure of Nb-dopedTiO2. Physical Review B, 2000, 61, 13445-13457.	1.1	264
94	Theoretical Study of the Chemisorption of CO on Al2O3(0001). Inorganic Chemistry, 2000, 39, 5232-5237.	1.9	24
95	Organometallic Chemistry of Ph3PCCO. Synthesis, Characterization, X-ray Structure Determination, and Density Functional Study of the First Stable Bis-Î·1-ketenyl Complex,trans-[PtCl2{Î·1-C(PPh3)CO}2]. Organometallics, 2000, 19, 1373-1383.	1.1	27
96	A theoretical study of the H2O and H2S chemisorption on Cu2O(111). Applied Surface Science, 1999, 142, 164-168.	3.1	44
97	A theoretical investigation of the relaxation effects induced on the ZnO(101Ì„0) surface by the chemisorption of H2 and CO. Applied Surface Science, 1999, 142, 192-195.	3.1	15
98	Density functional studies of molecular chemisorption on TiO2 (110). Applied Surface Science, 1999, 142, 196-199.	3.1	34
99	A comparative study of the NH3 chemisorption on ZnO(101Ì„0) and Cu2O(111) non-polar surfaces. Chemical Physics Letters, 1999, 300, 403-408.	1.2	23
100	Electronic structure of Nb impurities in and on TiO2. Physical Chemistry Chemical Physics, 1999, 1, 3793-3799.	1.3	20
101	Experimental and Theoretical Investigation of the Molecular and Electronic Structure of [Zn4(Î¼4-S){Î¼-S2As(CH3)2}6] and [Cd4(Î¼4-S){Î¼-S2As(CH3)2}6]:Â Two Possible Molecular Models of Extended Metal Chalcogenide Semiconductorsâ€. Inorganic Chemistry, 1999, 38, 1145-1152.	1.9	16
102	The adsorption of small molecules on the TiO2 anatase (101) surface by first-principles molecular dynamics. Surface Science, 1998, 402-404, 219-222.	0.8	88
103	LCAO-LDA Study of the chemisorption of formate on Cu(110) and Ag(110) surfaces. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 797-804.	1.7	8
104	Theoretical Investigation of the Chemisorption of H2and CO on the ZnO(101Ì„0) Surface. Inorganic Chemistry, 1998, 37, 5482-5490.	1.9	26
105	Molecular Chemisorption on TiO2(110):Â A Local Point of View. Journal of Physical Chemistry B, 1998, 102, 10745-10752.	1.2	91
106	Structure and Energetics of Water Adsorbed atTiO2Anatase (101) and (001) Surfaces. Physical Review Letters, 1998, 81, 2954-2957.	2.9	883
107	An Experimental and Theoretical Study of the Electronic Structure of Zinc Thiophenolate-Capped Clusters. Inorganic Chemistry, 1997, 36, 4707-4716.	1.9	37
108	An LCAO-LDF study of the chemisorption of H2O and H2S on ZnO(0001) and ZnO(101Ì„0). Surface Science, 1997, 377-379, 587-591.	0.8	50

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109	H2 adsorption/desorption at Si(111)-(7 Ã— 7): a density functional study. Surface Science, 1997, 383, L779-L784.	0.8	18
110	A theoretical study of the CO and NO chemisorption on Cu2O(111). Surface Science, 1997, 387, L1079-L1084.	0.8	32
111	A comparative study of CO and NO chemisorption on Cu2O(111) and Ag2O(111) non-polar surfaces. Chemical Physics Letters, 1997, 280, 53-58.	1.2	32
112	A LCAO-LDF study of Brâ^…nsted acids chemisorption on ZnO(0001). Surface Science, 1996, 352-354, 341-345.	0.8	9
113	An experimental and theoretical study of the interaction of CH3OH and CH3SH with ZnO. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 3247.	1.7	23
114	Binding Sites, Migration Paths, and Barriers for Hydrogen on Si(111)-(7 Ã— 7). Physical Review Letters, 1996, 76, 3662-3662.	2.9	4
115	A molecular cluster approach to the study of the bonding of CO and NH3 to a d10 ion on ZnO(0001) and CuCl(111). Inorganica Chimica Acta, 1995, 235, 151-158.	1.2	15
116	Density functional study of H2 desorption from monohydride and dihydride Si(100) surfaces. Chemical Physics Letters, 1995, 235, 334-340.	1.2	72
117	Binding Sites, Migration Paths, and Barriers for Hydrogen on Si(111)-(7Ã—7). Physical Review Letters, 1995, 75, 4756-4759.	2.9	72
118	Binding and diffusion of hydroxyl radicals on Si(100): A first-principles study. Physical Review B, 1995, 52, 5885-5889.	1.1	30
119	A theoretical investigation of BrÃ¸nsted acids chemisorption on ZnO(0001). Surface Science, 1995, 343, 115-132.	0.8	16
120	A theoretical and experimental investigation of the electronic structure of alpha -Fe2O3thin films. Journal of Physics Condensed Matter, 1995, 7, L299-L305.	0.7	15
121	Pairing of hydrogen atoms on the Si(100)-(2Ã—1) surface: The role of interactions among dimers. Physical Review B, 1994, 49, 11191-11195.	1.1	50
122	Surface carboxylate species on Cu(100) studied by angle-scanned photoelectron diffraction and LCAO-LDF calculations. Surface Science, 1994, 315, 309-322.	0.8	32
123	Coordination chemistry of CO and NH3 on CuCl(111): an experimental and theoretical study of the CO and NH3 bonding to a d10 ion. Surface Science, 1994, 317, 422-436.	0.8	20
124	A LCAO-LDF study of formate chemisorption on Cu(100). Surface Science, 1994, 307-309, 95-100.	0.8	23
125	Coordination chemistry of CO and NH3 on ZnO(0001): a molecular cluster study of the CO and NH3 bonding interaction with a d10 ion. Surface Science, 1994, 303, 125-138.	0.8	34
126	A LCAO-LDF study of CO and NH3 chemisorption on ZnO(0001). Surface Science, 1994, 307-309, 1182-1187.	0.8	16

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127	Energetics of atomic hydrogen diffusion on Si(100). Surface Science Letters, 1993, 289, L625-L630.	0.1	1
128	Energetics of atomic hydrogen diffusion on Si(100). Surface Science, 1993, 289, L625-L630.	0.8	48
129	Molecular-cluster model of the electronic structure of substitutional copper in zinc oxide. Journal of Materials Chemistry, 1993, 3, 53.	6.7	2
130	Zn4O(O2CNEt2)6: a further molecular model of ZnO. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 4363.	1.7	13
131	Experimental investigation of the electronic structures of enneacarbonylbis(.mu.3-X-methylidyne)triiron complexes (X = H, F, Cl, Br) by means of He I/He II gas-phase UV photoelectron spectroscopy. Inorganic Chemistry, 1993, 32, 1383-1388.	1.9	3
132	Theoretical study ofSiH3-defect stability and formation on the H-saturated Si(100)1Ã—1 surface. Physical Review B, 1992, 46, 4348-4351.	1.1	29
133	Hexakis(acetato)oxotetrazinc, a well-tailored molecular model of zinc oxide. An experimental and theoretical investigation of the electronic structure of Zn4O(acetate)6 and ZnO by means of UV and x-ray photoelectron spectroscopies and first principle local density molecular cluster calculations. Inorganic Chemistry, 1992, 31, 1558-1565.	1.9	130
134	A theoretical investigation of the electronic structure, hyperfine properties and binding energies of muonium centres in cuprous chloride. Chemical Physics, 1992, 159, 365-375.	0.9	2
135	Experimental and theoretical investigation of the electronic structure of two isoelectronic binuclear clusters. UV-PES and DV-X.alpha. study of ruthenium ethanediyldiamido carbonyl, Ru2(CO)6[.mu.,.mu.'-N(R)CH2CH2N(R)], and iron ruthenium ethanediyldiamido carbonyl, FeRu(CO)6[.mu.,.mu.'-N(R)CH2CH2N(R)]. Inorganic Chemistry, 1991, 30, 1906-1911.	1.9	6
136	A theoretical investigation of the hyperfine properties of normal and anomalous muonium in elemental semiconductors: Diamond, silicon and germanium. Chemical Physics, 1991, 154, 385-393.	0.9	8
137	A molecular cluster approach to the electronic structure of anomalous muonium in diamond. Chemical Physics, 1990, 148, 183-192.	0.9	2
138	Synthesis and reactivity of dimethylindium derivatives: molecular and electronic structure of bis(Î¼-diethylamido)-tetramethyldi-indium(III). Inorganica Chimica Acta, 1990, 170, 95-101.	1.2	11
139	Electronic structure of Ru3(CO)6(CH3Cî—»CHCH = NC3H7-i)2 as indicated by UV-photoelectron spectroscopy and DV-XÎ± quantum mechanical calculations. Journal of Organometallic Chemistry, 1990, 396, 73-81.	0.8	5
140	Molecular cluster model of the electronic structure of substitutional impurities in gallium arsenide. Chemistry of Materials, 1989, 1, 587-591.	3.2	3
141	Ruthenium carbonyl 1,4-diaza-1,3-butadiene (R-DAB) complexes. A theoretical and experimental investigation of the electronic structure of Ru2(CO)4(R-DAB)(.mu.-CO) and Ru2(CO)4(R-DAB)(.mu.-HC.tplbond.CH). Journal of the American Chemical Society, 1988, 110, 1775-1781.	6.6	7
142	Combined UV-PES and theoretical study of binuclear M2(CO)6(C4H4) complexes (M = Fe, Ru, Os). Inorganic Chemistry, 1987, 26, 2041-2046.	1.9	16
143	An accurate DV XÎ± investigation of the electronic structure of bis (2,4-pentanedionato) palladium(II). Chemical Physics Letters, 1987, 141, 193-197.	1.2	3
144	Electronic structure of bimetallic "flyover-bridge" derivatives. UV-PES and ab initio study of [cyclic] 511-514.	1.9	6

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145	A DV-XÎ± theoretical investigation of the electronic structure of some tris(cyclopentadienyl) complexes of U(IV). Inorganica Chimica Acta, 1986, 121, L23-L25.	1.2	7
146	Structure of (Z)-N-benzoyl-Î±,Î²-dehydroleucine. Acta Crystallographica Section C: Crystal Structure Communications, 1986, 42, 1178-1181.	0.4	6
147	Conformational and electronic effects in dehydroaminoacid derivatives. Journal of Molecular Structure, 1986, 141, 415-418.	1.8	0
148	Helium(He I and He II) photoelectron spectra of nickel(II), palladium(II) and platinum(II) diethyldithiocarbamate complexes. Inorganic Chemistry, 1984, 23, 702-706.	1.9	14