Louis Noodleman

List of Publications by Year in Descending Order

126 papers	13,044 citations	52 h-index	114 g-index
137 ext. papers	13,856 ext. citations	8 avg, IF	6.26 L-index

#	Paper	IF	Citations
126	Stereoelectronic effects in stabilizing protein-N-glycan interactions revealed by experiment and machine learning. *Nature Chemistry*, **2021**, 13, 480-487	17.6	3
125	Sulfur [F]Fluoride Exchange Click Chemistry Enabled Ultrafast Late-Stage Radiosynthesis. *Journal of the American Chemical Society*, **2021**, 143, 3753-3763	16.4	24
124	A Water Molecule Residing in the Fe□□Cu Dinuclear Center of the Resting Oxidized as-Isolated Cytochrome Oxidase: A Density Functional Study. *Inorganic Chemistry*, **2020**, 59, 8906-8915	5.1	6
123	Coupled transport of electrons and protons in a bacterial cytochrome oxidase-DFT calculated properties compared to structures and spectroscopies. *Physical Chemistry Chemical Physics*, **2020**, 22, 26652-26668	3.6	4
122	DFT Fe-O/O-O Vibrational Frequency Calculations over Catalytic Reaction Cycle States in the Dinuclear Center of Cytochrome Oxidase. *Inorganic Chemistry*, **2019**, 58, 13933-13944	5.1	7
121	The cytochrome b lysine 329 residue is critical for ubihydroquinone oxidation and proton release at the Q site of bacterial cytochrome bc. *Biochimica Et Biophysica Acta - Bioenergetics*, **2019**, 1860, 167-179	4.6	1
120	A Water Dimer Shift Activates a Proton Pumping Pathway in the P -> F Transition of ba Cytochrome c Oxidase. *Inorganic Chemistry*, **2018**, 57, 1048-1059	5.1	7
119	Water exit pathways and proton pumping mechanism in B-type cytochrome c oxidase from molecular dynamics simulations. *Biochimica Et Biophysica Acta - Bioenergetics*, **2016**, 1857, 1594-1606	4.6	12
118	The M□ssbauer Parameters of the Proximal Cluster of Membrane-Bound Hydrogenase Revisited: A Density Functional Theory Study. *Journal of Chemical Theory and Computation*, **2016**, 12, 174-87	6.4	10
117	Metalloproteins: Mapping elusive electron density. *Nature Chemical Biology*, **2016**, 12, 391-2	11.7	4
116	A broken-symmetry density functional study of structures, energies, and protonation states along the catalytic O-O bond cleavage pathway in ba3 cytochrome c oxidase from Thermus thermophilus. *Physical Chemistry Chemical Physics*, **2016**, 18, 21162-71	3.6	18
115	Data for molecular dynamics simulations of B-type cytochrome c oxidase with the Amber force field. *Data in Brief*, **2016**, 8, 1209-14	1.2	8
114	Broken-Symmetry DFT Computations for the Reaction Pathway of IspH, an Iron-Sulfur Enzyme in Pathogenic Bacteria. *Inorganic Chemistry*, **2015**, 54, 6439-61	5.1	11
113	Broken Symmetry DFT Calculations/Analysis for Oxidized and Reduced Dinuclear Center in Cytochrome c Oxidase: Relating Structures, Protonation States, Energies, and M□ssbauer Properties in ba3 Thermus thermophilus. *Inorganic Chemistry*, **2015**, 54, 7272-90	5.1	17
112	Electronic Structure, Bonding, Spin Coupling, and Energetics of Polynuclear Iron□Sulfur Clusters □A Broken Symmetry Density Functional Theory Perspective **2015**, 297-325		2
111	A fluorogenic aryl fluorosulfate for intraorganellar transthyretin imaging in living cells and in Caenorhabditis elegans. *Journal of the American Chemical Society*, **2015**, 137, 7404-14	16.4	65
110	EXAFS simulation refinement based on broken-symmetry DFT geometries for the Mn(IV)-Fe(III) center of class I RNR from Chlamydia trachomatis. *Dalton Transactions*, **2014**, 43, 576-83	4.3	3

109	Linking chemical electron-proton transfer to proton pumping in cytochrome c oxidase: broken-symmetry DFT exploration of intermediates along the catalytic reaction pathway of the iron-copper dinuclear complex. *Inorganic Chemistry*, **2014**, 53, 6458-72	5.1	30
108	Use of Broken-Symmetry Density Functional Theory To Characterize the IspH Oxidized State: Implications for IspH Mechanism and Inhibition. *Journal of Chemical Theory and Computation*, **2014**, 10, 3871-3884	6.4	13
107	Density functional study for the bridged dinuclear center based on a high-resolution X-ray crystal structure of ba3 cytochrome c oxidase from Thermus thermophilus. *Inorganic Chemistry*, **2013**, 52, 14072-88	5.1	19
106	Modeling the MoFe nitrogenase system with broken symmetry density functional theory. *Methods in Molecular Biology*, **2011**, 766, 293-312	1.4	15
105	Calibration of DFT Functionals for the Prediction of Fe Mössbauer Spectral Parameters in Iron-Nitrosyl and Iron-Sulfur Complexes: Accurate Geometries Prove Essential. *Journal of Chemical Theory and Computation*, **2011**, 7, 3232-3247	6.4	59
104	Geometric and electrostatic study of the [4Fe-4S] cluster of adenosine-5Pphosphosulfate reductase from broken symmetry density functional calculations and extended X-ray absorption fine structure spectroscopy. *Inorganic Chemistry*, **2011**, 50, 6610-25	5.1	24
103	Mössbauer properties of the diferric cluster and the differential iron(II)-binding affinity of the iron sites in protein R2 of class Ia Escherichia coli ribonucleotide reductase: a DFT/electrostatics study. *Dalton Transactions*, **2011**, 40, 11164-75	4.3	10
102	Correction to Density Functional Theory Calculations on Mo ssbauer Parameters of Nonheme Iron Nitrosyls. *Inorganic Chemistry*, **2011**, 50, 4221-4221	5.1	3
101	DFT calculations for intermediate and active states of the diiron center with a tryptophan or tyrosine radical in Escherichia coli ribonucleotide reductase. *Inorganic Chemistry*, **2011**, 50, 2302-20	5.1	23
100	Density functional theory analysis of structure, energetics, and spectroscopy for the Mn-Fe active site of Chlamydia trachomatis ribonucleotide reductase in four oxidation states. *Inorganic Chemistry*, **2010**, 49, 7266-81	5.1	29
99	Quantum cluster size and solvent polarity effects on the geometries and Mössbauer properties of the active site model for ribonucleotide reductase intermediate X: a density functional theory study. *Theoretical Chemistry Accounts*, **2010**, 125, 305-317	1.9	21
98	Spin coupling in Roussin's red and black salts. *Chemistry - A European Journal*, **2010**, 16, 10397-408	4.8	31
97	Density functional theory calculations on Mössbauer parameters of nonheme iron nitrosyls. *Inorganic Chemistry*, **2009**, 48, 9155-65	5.1	51
96	DFT calculations of comparative energetics and ENDOR/Mössbauer properties for two protonation states of the iron dimer cluster of ribonucleotide reductase intermediate X. *Dalton Transactions*, **2009**, 6045-57	4.3	24
95	Broken Symmetry States of IronSulfur Clusters **2009**,		3
94	IronSulfur Clusters: Properties and Functions **2008**, 1		2
93	Structural model studies for the peroxo intermediate P and the reaction pathway from P-->Q of methane monooxygenase using broken-symmetry density functional calculations. *Inorganic Chemistry*, **2008**, 47, 2975-86	5.1	52
92	Toward a chemical mechanism of proton pumping by the B-type cytochrome c oxidases: application of density functional theory to cytochrome ba3 of Thermus thermophilus. *Journal of the American Chemical Society*, **2008**, 130, 15002-21	16.4	60

91	Ligand-bound S = 1/2 FeMo-cofactor of nitrogenase: hyperfine interaction analysis and implication for the central ligand X identity. *Inorganic Chemistry*, **2008**, 47, 6162-72	5.1	51
90	Structural Model Studies for the High-Valent Intermediate Q of Methane Monooxygenase from Broken-Symmetry Density Functional Calculations. *Inorganica Chimica Acta*, **2008**, 361, 973-986	2.7	55
89	Testing if the interstitial atom, X, of the nitrogenase molybdenum-iron cofactor is N or C: ENDOR, ESEEM, and DFT studies of the S = 3/2 resting state in multiple environments. *Inorganic Chemistry*, **2007**, 46, 11437-49	5.1	77
88	Experimental and DFT studies: novel structural modifications greatly enhance the solvent sensitivity of live cell imaging dyes. *Journal of Physical Chemistry A*, **2007**, 111, 10849-60	2.8	20
87	Seven clues to the origin and structure of class-I ribonucleotide reductase intermediate X. *Journal of Inorganic Biochemistry*, **2006**, 100, 771-9	4.2	28
86	DFT calculations of 57Fe Mössbauer isomer shifts and quadrupole splittings for iron complexes in polar dielectric media: applications to methane monooxygenase and ribonucleotide reductase. *Journal of Computational Chemistry*, **2006**, 27, 1292-306	3.5	52
85	Density functional theory study of Fe(IV) d-d optical transitions in active-site models of class I ribonucleotide reductase intermediate X with vertical self-consistent reaction field methods. *Inorganic Chemistry*, **2006**, 45, 8533-42	5.1	26
84	Structure, redox, pKa, spin. A golden tetrad for understanding metalloenzyme energetics and reaction pathways. *Journal of Biological Inorganic Chemistry*, **2006**, 11, 674-94	3.7	80
83	Active site structure of class I ribonucleotide reductase intermediate X: a density functional theory analysis of structure, energetics, and spectroscopy. *Journal of the American Chemical Society*, **2005**, 127, 15778-90	16.4	62
82	Copper(I)-catalyzed synthesis of azoles. DFT study predicts unprecedented reactivity and intermediates. *Journal of the American Chemical Society*, **2005**, 127, 210-6	16.4	1311
81	On the role of the conserved aspartate in the hydrolysis of the phosphocysteine intermediate of the low molecular weight tyrosine phosphatase. *Journal of the American Chemical Society*, **2004**, 126, 12677-84	16.4	19
80	Nornicotine aqueous aldol reactions: synthetic and theoretical investigations into the origins of catalysis. *Journal of Organic Chemistry*, **2004**, 69, 6603-9	4.2	66
79	Density functional study of a micro-1,1-carboxylate bridged Fe(III)-O-Fe(IV) model complex. 2. Comparison with ribonucleotide reductase intermediate X. *Inorganic Chemistry*, **2004**, 43, 613-21	5.1	21
78	Quantum chemical studies of intermediates and reaction pathways in selected enzymes and catalytic synthetic systems. *Chemical Reviews*, **2004**, 104, 459-508	68.1	331
77	Density Functional Vertical Self-Consistent Reaction Field Theory for Solvatochromism Studies of Solvent-Sensitive Dyes. *Journal of Physical Chemistry A*, **2004**, 108, 3545-3555	2.8	38
76	Calculating the electron paramagnetic resonance parameters of exchange coupled transition metal complexes using broken symmetry density functional theory: application to a MnIII/MnIV model compound. *Journal of the American Chemical Society*, **2004**, 126, 2613-22	16.4	176
75	Temperature-dependent behavior of protein-chromophore interactions: a theoretical study of a blue fluorescent antibody. *ChemPhysChem*, **2003**, 4, 848-55	3.2	5
74	A theoretical study of the UV/visible absorption and emission solvatochromic properties of solvent-sensitive dyes. *ChemPhysChem*, **2003**, 4, 1084-94	3.2	75

73	Density functional and reduction potential calculations of Fe4S4 clusters. *Journal of the American Chemical Society*, **2003**, 125, 1923-36	16.4	189
72	The circumsphere as a tool to assess distortion in [4Fe-4S] atom clusters. *Journal of Biological Inorganic Chemistry*, **2003**, 8, 519-526	3.7	18
71	Structural, spectroscopic, and redox consequences of a central ligand in the FeMoco of nitrogenase: a density functional theoretical study. *Journal of the American Chemical Society*, **2003**, 125, 8377-83	16.4	133
70	A density functional evaluation of an Fe(III)-Fe(IV) model diiron cluster: comparisons with ribonucleotide reductase intermediate X. *Inorganic Chemistry*, **2003**, 42, 2751-8	5.1	37
69	Density functional theory study of the intramolecular [2 + 3] cycloaddition of azide to nitriles. *Journal of Organic Chemistry*, **2003**, 68, 9076-80	4.2	33
68	Photoisomerization and proton transfer in photoactive yellow protein. *Journal of the American Chemical Society*, **2003**, 125, 8186-94	16.4	54
67	Theoretical examination of Mg(2+)-mediated hydrolysis of a phosphodiester linkage as proposed for the hammerhead ribozyme. *Journal of the American Chemical Society*, **2003**, 125, 9861-7	16.4	35
66	DFT calculations of isomer shifts and quadrupole splitting parameters in synthetic iron-oxo complexes: applications to methane monooxygenase and ribonucleotide reductase. *Inorganic Chemistry*, **2003**, 42, 5244-51	5.1	40
65	Why is tetrazole formation by addition of azide to organic nitriles catalyzed by zinc(II) salts?. *Journal of the American Chemical Society*, **2003**, 125, 9983-7	16.4	305
64	Symmetry and bonding in metalloporphyrins. A modern implementation for the bonding analyses of five- and six-coordinate high-spin iron(III)-porphyrin complexes through density functional calculation and NMR spectroscopy. *Journal of the American Chemical Society*, **2003**, 125, 6774-83	16.4	70
63	Density functional studies of the ground- and excited-state potential-energy curves of stilbene cis-trans isomerization. *ChemPhysChem*, **2002**, 3, 167-78	3.2	65
62	Insights into properties and energetics of iron-sulfur proteins from simple clusters to nitrogenase. *Current Opinion in Chemical Biology*, **2002**, 6, 259-73	9.7	117
61	Density functional calculation of p K(a) values and redox potentials in the bovine Rieske iron-sulfur protein. *Journal of Biological Inorganic Chemistry*, **2002**, 7, 632-9	3.7	103
60	FeMo cofactor of nitrogenase: energetics and local interactions in the protein environment. *Journal of Biological Inorganic Chemistry*, **2002**, 7, 735-49	3.7	40
59	Density functional and electrostatics study of oxidized and reduced ribonucleotide reductase; comparisons with methane monooxygenase. *Journal of Biological Inorganic Chemistry*, **2002**, 7, 799-809	3.7	10
58	Mechanisms of tetrazole formation by addition of azide to nitriles. *Journal of the American Chemical Society*, **2002**, 124, 12210-6	16.4	273
57	A structural model for the high-valent intermediate Q of methane monooxygenase from broken-symmetry density functional and electrostatics calculations. *Journal of the American Chemical Society*, **2002**, 124, 5890-4	16.4	74
56	Density functional study of the mechanism of a tyrosine phosphatase: I. Intermediate formation. *Journal of the American Chemical Society*, **2002**, 124, 10225-35	16.4	41

55	Coupled redox potentials in manganese and iron superoxide dismutases from reaction kinetics and density functional/electrostatics calculations. *Inorganic Chemistry*, **2002**, 41, 205-18	5.1	64
54	Binding modes for the first coupled electron and proton addition to FeMoco of nitrogenase. *Journal of the American Chemical Society*, **2002**, 124, 4546-7	16.4	40
53	Metal substitution in the active site of nitrogenase MFe(7)S(9) (M = Mo(4+), V(3+), Fe(3+)). *Inorganic Chemistry*, **2002**, 41, 5744-53	5.1	48
52	Relative Acidities of Ortho-Substituted Phenols, as Models for Modified Tyrosines in Proteins. *Journal of Physical Chemistry A*, **2002**, 106, 8757-8761	2.8	40
51	Multiple reactive immunization towards the hydrolysis of organophosphorus nerve agents: hapten design and synthesis. *Bioorganic and Medicinal Chemistry*, **2001**, 9, 3185-95	3.4	8
50	FeMo cofactor of nitrogenase: a density functional study of states M(N), M(OX), M(R), and M(I). *Journal of the American Chemical Society*, **2001**, 123, 12392-410	16.4	152
49	Density functional studies of oxidized and reduced methane monooxygenase. Optimized geometries and exchange coupling of active site clusters. *Inorganic Chemistry*, **2001**, 40, 5251-66	5.1	30
48	Energetics of oxidized and reduced methane monooxygenase active site clusters in the protein environment. *Inorganic Chemistry*, **2001**, 40, 5267-78	5.1	25
47	Modern Computational Approaches to Modeling Polynuclear Transition Metal Complexes **2000**, 19-47		2
46	CuZn Superoxide Dismutase Geometry Optimization, Energetics, and Redox Potential Calculations by Density Functional and Electrostatic Methods. *Inorganic Chemistry*, **1999**, 38, 940-950	5.1	75
45	Density Functional and Electrostatic Calculations of Manganese Superoxide Dismutase Active Site Complexes in Protein Environments. *Inorganic Chemistry*, **1999**, 38, 929-939	5.1	64
44	Incorporating Protein Environments in Density Functional Theory: A Self-Consistent Reaction Field Calculation of Redox Potentials of [2Fe2S] Clusters in Ferredoxin and Phthalate Dioxygenase Reductase. *Journal of Physical Chemistry A*, **1998**, 102, 6311-6324	2.8	112
43	Electronic Structure Calculations: Density Functional Methods for Spin Polarization, Charge Transfer, and Solvent Effects in Transition Metal Complexes. *ACS Symposium Series*, **1998**, 179-196	0.4	11
42	Density Functional Study of the Valence-Tautomeric Interconversion Low-Spin [CoIII(SQ)(Cat)(phen)] ? High-Spin [CoII(SQ)2(phen)]. *Inorganic Chemistry*, **1997**, 36, 3966-3984	5.1	132
41	Density Functional Study on the Electronic Structures of Model Peroxidase Compounds I and II. *Journal of the American Chemical Society*, **1997**, 119, 11442-11451	16.4	88
40	Density Functional Calculations of Electronic Structure, Charge Distribution, and Spin Coupling in Manganese-Oxo Dimer Complexes. *Inorganic Chemistry*, **1997**, 36, 1198-1217	5.1	94
39	Calculation of Redox Potentials and pKa Values of Hydrated Transition Metal Cations by a Combined Density Functional and Continuum Dielectric Theory. *Inorganic Chemistry*, **1996**, 35, 4694-4702	5.1	215
38	Density-Functional and Electrostatic Calculations for a Model of a Manganese Superoxide Dismutase Active Site in Aqueous Solution. *The Journal of Physical Chemistry*, **1996**, 100, 13498-13505		42

37	Valence electron delocalization in polynuclear iron-sulfur clusters. *Journal of Biological Inorganic Chemistry*, **1996**, 1, 177-182	3.7	49
36	Using antibodies to perturb the coordination sphere of a transition metal complex. *Nature*, **1996**, 382, 339-41	50.4	24
35	Density-functional calculations of spin coupling in [Fe4S4]3+ clusters. *International Journal of Quantum Chemistry*, **1995**, 56, 95-102	2.1	31
34	Orbital interactions, electron delocalization and spin coupling in iron-sulfur clusters. *Coordination Chemistry Reviews*, **1995**, 144, 199-244	23.2	683
33	Spin Densities and Spin Coupling in Iron-Sulfur Clusters: A New Analysis of Hyperfine Coupling Constants. *Inorganic Chemistry*, **1995**, 34, 4347-4359	5.1	131
32	Incorporating Solvation Effects into Density Functional Electronic Structure Calculations. *The Journal of Physical Chemistry*, **1994**, 98, 11059-11068		158
31	Density Functional/Poisson-Boltzmann Calculations of Redox Potentials for Iron-Sulfur Clusters. *Journal of the American Chemical Society*, **1994**, 116, 11898-11914	16.4	272
30	Analysis of the 57Fe Hyperfine Coupling Constants and Spin States in Nitrogenase P-Clusters. *Inorganic Chemistry*, **1994**, 33, 4819-4830	5.1	51
29	Density-Functional Theory of Spin Polarization and Spin Coupling in Iron Sulfur Clusters. *Advances in Inorganic Chemistry*, **1992**, 38, 423-470	2.1	513
28	LCAO X.alpha. calculation of the magnetic exchange interactions in a manganese MnIVMn3III cubane complex: relevance to the water oxidation center of photosystem II. *Journal of the American Chemical Society*, **1992**, 114, 6109-6119	16.4	48
27	Fe(CO)4XXX radical anion: theoretical study of the electronic structure and magnetic properties. *Computational and Theoretical Chemistry*, **1991**, 226, 251-263		3
26	Exchange coupling and resonance delocalization in reduced iron-sulfur [Fe4S4]+ and iron-selenium [Fe4Se4]+ clusters. 2. A generalized nonlinear model for spin-state energies and EPR and hyperfine properties. *Inorganic Chemistry*, **1991**, 30, 256-264	5.1	64
25	Exchange coupling and resonance delocalization in reduced iron-sulfur [Fe4S4]+ and iron-selenium [Fe4Se4]+ clusters. 1. Basic theory of spin-state energies and EPR and hyperfine properties. *Inorganic Chemistry*, **1991**, 30, 246-256	5.1	77
24	Local Density Functional Approaches to Spin Coupling in Transition Metal Clusters **1991**, 109-123		1
23	Magnetic studies of the high-potential protein model [Fe4S4(S-2,4,6-(iso-Pr)3C6H2)4]- in the [Fe4S4]3+ oxidized state. *Inorganic Chemistry*, **1990**, 29, 4288-4292	5.1	51
22	Modeling of palmitate transport in the heart. *Molecular and Cellular Biochemistry*, **1989**, 88, 51-8	4.2	60
21	Electronic structure in broken space- and spin- symmetry : applications to Fe-s proteins and clusters. *Journal De Chimie Physique Et De Physico-Chimie Biologique*, **1989**, 86, 743-755		13
20	A model for the spin states of high-potential iron-sulfur [Fe4S4]3+ proteins. *Inorganic Chemistry*, **1988**, 27, 3677-3679	5.1	108

19	Characterization of [4Fe-4Se]2+/3+ high-potential iron-sulfur protein from Chromatium vinosum. *Biochemistry*, **1988**, 27, 8712-8719	3.2	26
18	Broken symmetry analysis of spin coupling in iron-sulfur clusters. *Journal of the American Chemical Society*, **1988**, 110, 1001-1005	16.4	204
17	Ligand spin polarization and antiferromagnetic coupling in transition metal dimers. *Chemical Physics*, **1986**, 109, 131-143	2.3	815
16	Models for ferredoxins: electronic structures of iron-sulfur clusters with one, two, and four iron atoms. *Journal of the American Chemical Society*, **1985**, 107, 3418-3426	16.4	274
15	Electronic structure, magnetic properties, ESR, and optical spectra for 2-iron ferredoxin models by LCAO-X.alpha. valence bond theory. *Journal of the American Chemical Society*, **1984**, 106, 2316-2327	16.4	479
14	Broken symmetry effects in the He(I) valence photoelectron spectrum of Se(CN)2. *Molecular Physics* , **1982**, 46, 609-620	1.7	32
13	Symmetry breaking and ionization from symmetry equivalent inner shells and lone pairs in X□ theory. *Chemical Physics*, **1982**, 64, 159-166	2.3	58
12	Valence bond description of antiferromagnetic coupling in transition metal dimers. *Journal of Chemical Physics*, **1981**, 74, 5737-5743	3.9	2090
11	Electronic structure of 2-Fe ferredoxin models by X.alpha. valence bond theory. *Journal of the American Chemical Society*, **1980**, 102, 4279-4282	16.4	97
10	Selective naked-cluster cryophotochemistry and SCF-X.alpha.-SW calculations for copper (Cu2) and silver (Ag2). *Journal of the American Chemical Society*, **1979**, 101, 3504-3511	16.4	54
9	Trimethylamine, trisilylamine, and trigermylamine: a comparative study of ionization energies, charge distribution, and bonding. *Inorganic Chemistry*, **1979**, 18, 354-360	5.1	18
8	The X□valence bond theory of weak electronic coupling. Application to the low-lying states of Mo2Cl84□*Journal of Chemical Physics*, **1979**, 70, 4903-4906	3.9	370
7	Ionization energies and electronic structure of N3P3Cl6 as determined by UV photoelectron spectroscopy and the X□scattered wave method. *Chemical Physics Letters*, **1978**, 58, 252-258	2.5	4
6	X.alpha. scattered-wave calculations of the electronic structures of sulfur dioxide and sulfuryl fluoride. Relationship to .pi. bonding in the cyclic phosphazenes. *Inorganic Chemistry*, **1978**, 17, 2709-2717	5.1	12
5	The electronic structure of tetraphosphorus trisulphide. *Canadian Journal of Chemistry*, **1977**, 55, 669-681	1.9	17
4	Local density of states calculated with the X□scattered wave method for some clusters of silver atoms. *Surface Science*, **1977**, 69, 714-720	1.8	10
3	X□scattered wave calculations of the ionisation energies of N3P3F6 and N4P4F8. *Chemical Physics Letters*, **1977**, 47, 265-268	2.5	11
2	A study of the core electron binding energies of ozone by x-ray photoelectron spectroscopy and the X□scattered wave method. *Chemical Physics Letters*, **1977**, 49, 213-217	2.5	24

1	The determination of optical absorption intensities using the X□scattered wave method. *Journal of Chemical Physics*, **1976**, 64, 2343	3.9	57