Jerry L Whitten

List of Publications by Year
in descending order

86	2,363	218677	214800
papers	citations	26 h-index	47 g-index

87	87	87	1416
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Understanding the electrospray ionization response factors of per- and poly-fluoroalkyl substances (PFAS). Analytical and Bioanalytical Chemistry, 2022, 414, 1227-1234.	3.7	8
2	Estimates of electron correlation based on density expansions. Journal of Chemical Physics, 2020, 153, 244103.	3.0	1
3	Prediction of many-electron wavefunctions using atomic potentials: extended basis sets and molecular dissociation. Physical Chemistry Chemical Physics, 2019, 21, 21541-21548.	2.8	4
4	Electronic and Structural Factors Controlling the Spin Orientations of Magnetic Ions. Inorganic Chemistry, 2019, 58, 11854-11874.	4.0	30
5	The Conceptual Dilemma of the One-Electron Picture in Describing the Uniaxial Magnetism at Linear Coordination Sites. European Journal of Inorganic Chemistry, 2019, 2019, 2630-2634.	2.0	3
6	Prediction of many-electron wavefunctions using atomic potentials: Refinements and extensions to transition metals and large systems. Journal of Chemical Physics, 2019, 150, 034107.	3.0	4
7	Electron correlation by polarization of interacting densities. Journal of Chemical Physics, 2017, 146, 064113.	3.0	4
8	Prediction of many-electron wavefunctions using atomic potentials. Journal of Chemical Physics, 2017, 146, 194109.	3.0	6
9	Adsorption of copper on a Î³-alumina support. Surface Science, 2016, 651, 22-27.	1.9	8
10	Electronic structure and spectra of (Cu₂O)_nâ€“H₂O complexes. Physical Chemistry Chemical Physics, 2015, 17, 428-433.	2.8	4
11	CI and DFT Studies of the Adsorption of the Nerve Agent Sarin on Surfaces. Journal of Physical Chemistry C, 2014, 118, 23042-23048.	3.1	17
12	Reaction pathways for butanoic acid decarboxylation on the (111) surface of a Pd nanoparticle. Surface Science, 2013, 607, 130-137.	1.9	14
13	Band-Edge Electronic States, and Pre-Existing Defects in Remote Plasma Deposited (RPD) GeO2 and SiO2. , 2012, , .		0
14	Theoretical Study of the Molecular and Electronic Structures of TiO₄H₄, Ti₂O₇H₆, and Ti₂O₆H₄. Journal of Physical Chemistry C, 2011, 115, 1635-1642.	3.1	7
15	Configuration interaction study of the ground and excited states of TiO2 ring structures. Journal of Chemical Physics, 2011, 134, 114701.	3.0	4
16	Dissociation of water on a palladium nanoparticle. International Journal of Quantum Chemistry, 2010, 110, 3072-3079.	2.0	12
17	Improving limits of detection for B-type natriuretic peptide using PC-IDMS: An application of the ALiPHAT strategy. Analyst, The, 2010, 135, 36-41.	3.5	20
18	Photoinduced dissociation of water adsorbed on a Ag cluster. Computational and Theoretical Chemistry, 2009, 903, 28-33.	1.5	4

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19	Evaluation of the ALiPHAT method for PC-IDMS and correlation of limits-of-detection with nonpolar surface area. Journal of the American Society for Mass Spectrometry, 2009, 20, 2006-2012.	2.8	15
20	Theoretical treatment of excited electronic states of adsorbates on metals: Electron attachment to CO2 adsorbed on K-modified Pt(111). Surface Science, 2008, 602, 834-842.	1.9	5
21	Photoinduced Dissociation of Water and Transport of Hydrogen between Silver Clusters. Journal of Physical Chemistry A, 2008, 112, 6358-6363.	2.5	7
22	Theoretical Study of the Photoinduced Câ^'H Bond Cleavage in Formaldehyde Adsorbed on the Ag(111) Surface. Journal of Physical Chemistry C, 2007, 111, 9914-9918.	3.1	1
23	Theoretical treatment of excited electronic states of adsorbates on metals: Electron attachment to CO2 adsorbed on Pt(111). Surface Science, 2007, 601, 3755-3759.	1.9	9
24	CO Adsorption on Ag(100) and Ag/MgO(100). Journal of Physical Chemistry B, 2006, 110, 11272-11276.	2.6	29
25	Weak Hydrogen Bonding Can Initiate Alkane Câ^'H Bond Activation in Acidic Zeolites. Journal of Physical Chemistry B, 2006, 110, 20762-20764.	2.6	17
26	Trends in adsorption of open-shell atoms and small molecular fragments on the Ag(111) surface. Surface Science, 2006, 600, 5104-5113.	1.9	23
27	Materials and Processes for High k Gate Stacks: Results from the FEP Transition Center. ECS Transactions, 2006, 3, 389-415.	0.5	2
28	Interaction of S, SH and H2S with Ag(100). Surface Science, 2005, 588, 83-91.	1.9	17
29	Theoretical Study of the CH2 + O Photodissociation of Formaldehyde Adsorbed on the Ag(111) Surface. Journal of Physical Chemistry B, 2005, 109, 18070-18080.	2.6	8
30	Adsorption of O, H, OH, and H2O on Ag(100). Journal of Physical Chemistry B, 2005, 109, 8852-8856.	2.6	38
31	Electronic structure of transition metal high-k dielectrics: interfacial band offset energies for microelectronic devices. Applied Surface Science, 2003, 212-213, 563-569.	6.1	21
32	Band offset energies in zirconium silicate Si alloys. Applied Surface Science, 2003, 216, 215-222.	6.1	7
33	A molecular orbital model for the electronic structure of transition metal atoms in silcate and aluminate alloys. Applied Surface Science, 2002, 190, 48-55.	6.1	1
34	A molecular orbital model for the electronic structure of transition metal atoms in silicate and aluminate alloys. Microelectronic Engineering, 2001, 59, 329-334.	2.4	19
35	Adsorption Energetics of NO and CO on Pt(111). Journal of Cluster Science, 1999, 10, 581-590.	3.3	6
36	Quantum Catalysis: The Modeling of Catalytic Transition States. ACS Symposium Series, 1999, , 2-17.	0.5	7

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37	Reaction and adsorption energetics of CN+Oâ†'OCN on nickel. Computational and Theoretical Chemistry, 1998, 458, 131-142.	1.5	13
38	Chemisorption of OCN on Ni(100) â€“ an ab initio study. Surface Science, 1998, 401, 312-321.	1.9	24
39	Energetics of adsorption and coadsorption of CN and O on Ni(100). Journal of Chemical Physics, 1997, 107, 8518-8524.	3.0	20
40	Energetics of Hydroxyl and Influence of Coadsorbed Oxygen on Metal Surfaces. Journal of Physical Chemistry B, 1997, 101, 4090-4096.	2.6	16
41	Adsorption of SH and OH and coadsorption of S, O and H on Ni(111). Surface Science, 1997, 370, 136-154.	1.9	54
42	Coadsorption of CO and CH3O on Ni(100). Surface Science, 1997, 375, 268-280.	1.9	15
43	Chemisorption of CNH2 and HCNH on the Ni(111) surface. Chemical Physics Letters, 1996, 251, 20-25.	2.6	22
44	Theoretical Adsorption Studies of HCN and HNC on Ni(111). The Journal of Physical Chemistry, 1996, 100, 5090-5097.	2.9	10
45	Ab initio studies of CN adsorbed on Ni(111). Journal of Chemical Physics, 1995, 103, 8756-8763.	3.0	37
46	Multiconfiguration selfâ€consistentâ€field treatment of H2 desorption from Si(100)â€2Ã—1H. Journal of Chemical Physics, 1995, 102, 3867-3872.	3.0	33
47	Adsorption of Formyl on Ni(100). Langmuir, 1995, 11, 853-859.	3.5	18
48	Ab initio chemisorption studies of H on Fe(110). Surface Science, 1995, 330, 255-264.	1.9	24
49	Integration of Plasma-Assisted and Rapid Thermal Processing for Low-Thermal Budget Preparation of Ultra-Thin Dielectrics for Stacked-Gate Device Structures. Japanese Journal of Applied Physics, 1994, 33, 7061-7070.	1.5	8
50	Bonding of carbon to nickel surfaces: effects of subsurface Na, H and C. Applied Surface Science, 1994, 75, 12-20.	6.1	8
51	Effects of oxygen on surface reconstruction of carbon. Applied Surface Science, 1994, 75, 45-50.	6.1	28
52	Adsorption of CH3O on Ni(111). Surface Science, 1994, 313, 295-307.	1.9	34
53	Chemisorption Studies of CH3S on Ni(111). Journal of the American Chemical Society, 1994, 116, 8200-8206.	13.7	23
54	Reaction of CH4 and CH3F with Si(111). Journal of Electron Spectroscopy and Related Phenomena, 1994, 69, 23-29.	1.7	5

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55	Effects of subsurface Na, H and C on the bonding of carbon to nickel surfaces. Surface Science Letters, 1993, 294, L945-L951.	0.1	0
56	Dissociative adsorption of H2 on Ni(111). Journal of Chemical Physics, 1993, 98, 5039-5049.	3.0	92
57	Effects of subsurface Na, H and C on the bonding of carbon to nickel surfaces. Surface Science, 1993, 294, L945-L951.	1.9	6
58	Reaction of CH4 with substitutional Fe/Ni(111). Surface Science, 1993, 289, 30-38.	1.9	6
59	Dissociative chemisorption of CH4 on Ni(111). Journal of Chemical Physics, 1992, 96, 5529-5537.	3.0	147
60	Ab initio studies of Si(100) surface reconstruction. Surface Science, 1992, 274, 106-112.	1.9	37
61	Effects of subsurface Na, H and C on CH3 adsorption on Ni(111). Surface Science, 1992, 277, L95-L99.	1.9	16
62	Effects of subsurface Na, H and C on CH3 adsorption on Ni(111). Surface Science Letters, 1992, 277, L95-L99.	0.1	1
63	Chemisorption of atomic H and CHx fragments on Ni(111). Surface Science, 1991, 255, 193-207.	1.9	88
64	The adsorption of benzene on Ni(111). Surface Science, 1991, 250, 147-158.	1.9	55
65	Ab initiostudies of silane decomposition on Si(100). Physical Review B, 1991, 44, 1741-1746.	3.2	25
66	Ab initio chemisorption studies of methyl on nickel(111). Journal of the American Chemical Society, 1991, 113, 6442-6449.	13.7	83
67	Multiparent configuration interaction calculations of low-lying states of O22+. Chemical Physics, 1990, 147, 115-119.	1.9	21
68	Influence of surface impurity on impact response of lattices. Journal of Applied Physics, 1990, 67, 1397-1407.	2.5	0
69	Adsorption of ammonia on nickel(111). The Journal of Physical Chemistry, 1990, 94, 6379-6383.	2.9	62
70	Reaction of Methane with Nickel [111] Surface. ACS Symposium Series, 1989, , 140-152.	0.5	5
71	Reaction of chemisorbed CH and H on nickel. Journal of Chemical Physics, 1989, 91, 126-136.	3.0	33
72	The adsorption of water and hydroxyl on Ni(lll). Surface Science, 1989, 223, 131-150.	1.9	95

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73	Collision-induced dissociation and ab initio studies of boron cluster ions: determination of structures and stabilities. The Journal of Physical Chemistry, 1988, 92, 5803-5812.	2.9	244
74	Chemisorption of hydrogen on the nickel (111) surface. Journal of Chemical Physics, 1988, 89, 5329-5334.	3.0	71
75	Ab initio evaluation of the Born correction, Born couplings, and higher derivative matrix elements with Gaussianâ€lobe orbitals. Journal of Chemical Physics, 1988, 88, 7662-7670.	3.0	6
76	The effect of hydrogen chemisorption on titanium surface bonding. Theoretica Chimica Acta, 1987, 72, 485-496.	0.8	46
77	Theoretical studies of interstitial hydrogen in titanium. Surface Science, 1985, 149, 273-284.	1.9	41
78	Iterative natural orbitals for configuration interaction using perturbation theory. Theoretica Chimica Acta, 1977, 44, 305-313.	0.8	6
79	Ab initio studies of molecules and concepts of molecular structure. Accounts of Chemical Research, 1973, 6, 238-245.	15.6	10
80	Study of Linear Stretch in Polyatomic Molecules: Accurate SCF MO Wavefunctions for CO2 and BeF2. Journal of Chemical Physics, 1967, 46, 1707-1716.	3.0	43
81	Theoretical Analysis of the Effects of Hydrogenation in Hydrocarbons: Accurate SCF MO Wavefunctions for C2H2, C2H4, and C2H6. Journal of Chemical Physics, 1967, 46, 2029-2039.	3.0	70
82	Geometry of Molecules. II. Diborane and Ethane. Journal of Chemical Physics, 1966, 45, 2835-2847.	3.0	49
83	Method for Computing Multicenter Oneâ€•and Twoâ€Electron Integrals. Journal of Chemical Physics, 1965, 43, S170-S171.	3.0	29
84	Helium Difluoride. Journal of the American Chemical Society, 1965, 87, 3769-3771.	13.7	8
85	Gaussian Expansion of Hydrogenâ€Atom Wavefunctions. Journal of Chemical Physics, 1963, 39, 349-352.	3.0	194
86	Chemical bonding and electronic structure of high-? transition metal dielectrics: applications to interfacial band offset energies and electronically active defects. , 0, , .		0