

# Jerry L Whitten

## List of Publications by Year in descending order

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86  
papers

2,363  
citations

218677

26  
h-index

214800

47  
g-index

87  
all docs

87  
docs citations

87  
times ranked

1416  
citing authors

#	ARTICLE	IF	CITATIONS
1	Collision-induced dissociation and ab initio studies of boron cluster ions: determination of structures and stabilities. <i>The Journal of Physical Chemistry</i> , 1988, 92, 5803-5812.	2.9	244
2	Gaussian Expansion of Hydrogen-Atom Wavefunctions. <i>Journal of Chemical Physics</i> , 1963, 39, 349-352.	3.0	194
3	Dissociative chemisorption of CH <sub>4</sub> on Ni(111). <i>Journal of Chemical Physics</i> , 1992, 96, 5529-5537.	3.0	147
4	The adsorption of water and hydroxyl on Ni(111). <i>Surface Science</i> , 1989, 223, 131-150.	1.9	95
5	Dissociative adsorption of H <sub>2</sub> on Ni(111). <i>Journal of Chemical Physics</i> , 1993, 98, 5039-5049.	3.0	92
6	Chemisorption of atomic H and CH <sub>x</sub> fragments on Ni(111). <i>Surface Science</i> , 1991, 255, 193-207.	1.9	88
7	Ab initio chemisorption studies of methyl on nickel(111). <i>Journal of the American Chemical Society</i> , 1991, 113, 6442-6449.	13.7	83
8	Chemisorption of hydrogen on the nickel (111) surface. <i>Journal of Chemical Physics</i> , 1988, 89, 5329-5334.	3.0	71
9	Theoretical Analysis of the Effects of Hydrogenation in Hydrocarbons: Accurate SCF MO Wavefunctions for C <sub>2</sub> H <sub>2</sub> , C <sub>2</sub> H <sub>4</sub> , and C <sub>2</sub> H <sub>6</sub> . <i>Journal of Chemical Physics</i> , 1967, 46, 2029-2039.	3.0	70
10	Adsorption of ammonia on nickel(111). <i>The Journal of Physical Chemistry</i> , 1990, 94, 6379-6383.	2.9	62
11	The adsorption of benzene on Ni(111). <i>Surface Science</i> , 1991, 250, 147-158.	1.9	55
12	Adsorption of SH and OH and coadsorption of S, O and H on Ni(111). <i>Surface Science</i> , 1997, 370, 136-154.	1.9	54
13	Geometry of Molecules. II. Diborane and Ethane. <i>Journal of Chemical Physics</i> , 1966, 45, 2835-2847.	3.0	49
14	The effect of hydrogen chemisorption on titanium surface bonding. <i>Theoretica Chimica Acta</i> , 1987, 72, 485-496.	0.8	46
15	Study of Linear Stretch in Polyatomic Molecules: Accurate SCF MO Wavefunctions for CO <sub>2</sub> and BeF <sub>2</sub> . <i>Journal of Chemical Physics</i> , 1967, 46, 1707-1716.	3.0	43
16	Theoretical studies of interstitial hydrogen in titanium. <i>Surface Science</i> , 1985, 149, 273-284.	1.9	41
17	Adsorption of O, H, OH, and H <sub>2</sub> O on Ag(100). <i>Journal of Physical Chemistry B</i> , 2005, 109, 8852-8856.	2.6	38
18	Ab initio studies of Si(100) surface reconstruction. <i>Surface Science</i> , 1992, 274, 106-112.	1.9	37

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19	Ab initio studies of CN adsorbed on Ni(111). <i>Journal of Chemical Physics</i> , 1995, 103, 8756-8763.	3.0	37
20	Adsorption of CH <sub>3</sub> O on Ni(111). <i>Surface Science</i> , 1994, 313, 295-307.	1.9	34
21	Reaction of chemisorbed CH and H on nickel. <i>Journal of Chemical Physics</i> , 1989, 91, 126-136.	3.0	33
22	Multiconfiguration self-consistent-field treatment of H <sub>2</sub> desorption from Si(100)-1H. <i>Journal of Chemical Physics</i> , 1995, 102, 3867-3872.	3.0	33
23	Electronic and Structural Factors Controlling the Spin Orientations of Magnetic Ions. <i>Inorganic Chemistry</i> , 2019, 58, 11854-11874.	4.0	30
24	Method for Computing Multicenter One- and Two-Electron Integrals. <i>Journal of Chemical Physics</i> , 1965, 43, S170-S171.	3.0	29
25	CO Adsorption on Ag(100) and Ag/MgO(100). <i>Journal of Physical Chemistry B</i> , 2006, 110, 11272-11276.	2.6	29
26	Effects of oxygen on surface reconstruction of carbon. <i>Applied Surface Science</i> , 1994, 75, 45-50.	6.1	28
27	Ab initio studies of silane decomposition on Si(100). <i>Physical Review B</i> , 1991, 44, 1741-1746.	3.2	25
28	Ab initio chemisorption studies of H on Fe(110). <i>Surface Science</i> , 1995, 330, 255-264.	1.9	24
29	Chemisorption of OCN on Ni(100) – an ab initio study. <i>Surface Science</i> , 1998, 401, 312-321.	1.9	24
30	Chemisorption Studies of CH <sub>3</sub> S on Ni(111). <i>Journal of the American Chemical Society</i> , 1994, 116, 8200-8206.	13.7	23
31	Trends in adsorption of open-shell atoms and small molecular fragments on the Ag(111) surface. <i>Surface Science</i> , 2006, 600, 5104-5113.	1.9	23
32	Chemisorption of CNH <sub>2</sub> and HCNH on the Ni(111) surface. <i>Chemical Physics Letters</i> , 1996, 251, 20-25.	2.6	22
33	Multiparent configuration interaction calculations of low-lying states of O <sub>2</sub> <sup>2+</sup> . <i>Chemical Physics</i> , 1990, 147, 115-119.	1.9	21
34	Electronic structure of transition metal high-k dielectrics: interfacial band offset energies for microelectronic devices. <i>Applied Surface Science</i> , 2003, 212-213, 563-569.	6.1	21
35	Energetics of adsorption and coadsorption of CN and O on Ni(100). <i>Journal of Chemical Physics</i> , 1997, 107, 8518-8524.	3.0	20
36	Improving limits of detection for B-type natriuretic peptide using PC-IDMS: An application of the ALiPHAT strategy. <i>Analyst</i> , 2010, 135, 36-41.	3.5	20

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37	A molecular orbital model for the electronic structure of transition metal atoms in silicate and aluminate alloys. <i>Microelectronic Engineering</i> , 2001, 59, 329-334.	2.4	19
38	Adsorption of Formyl on Ni(100). <i>Langmuir</i> , 1995, 11, 853-859.	3.5	18
39	Interaction of S, SH and H <sub>2</sub> S with Ag(100). <i>Surface Science</i> , 2005, 588, 83-91.	1.9	17
40	Weak Hydrogen Bonding Can Initiate Alkane C-H Bond Activation in Acidic Zeolites. <i>Journal of Physical Chemistry B</i> , 2006, 110, 20762-20764.	2.6	17
41	CI and DFT Studies of the Adsorption of the Nerve Agent Sarin on Surfaces. <i>Journal of Physical Chemistry C</i> , 2014, 118, 23042-23048.	3.1	17
42	Effects of subsurface Na, H and C on CH <sub>3</sub> adsorption on Ni(111). <i>Surface Science</i> , 1992, 277, L95-L99.	1.9	16
43	Energetics of Hydroxyl and Influence of Coadsorbed Oxygen on Metal Surfaces. <i>Journal of Physical Chemistry B</i> , 1997, 101, 4090-4096.	2.6	16
44	Coadsorption of CO and CH <sub>3</sub> O on Ni(100). <i>Surface Science</i> , 1997, 375, 268-280.	1.9	15
45	Evaluation of the ALiPHAT method for PC-IDMS and correlation of limits-of-detection with nonpolar surface area. <i>Journal of the American Society for Mass Spectrometry</i> , 2009, 20, 2006-2012.	2.8	15
46	Reaction pathways for butanoic acid decarboxylation on the (111) surface of a Pd nanoparticle. <i>Surface Science</i> , 2013, 607, 130-137.	1.9	14
47	Reaction and adsorption energetics of CN+O <sup>+</sup> OCN on nickel. <i>Computational and Theoretical Chemistry</i> , 1998, 458, 131-142.	1.5	13
48	Dissociation of water on a palladium nanoparticle. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 3072-3079.	2.0	12
49	Ab initio studies of molecules and concepts of molecular structure. <i>Accounts of Chemical Research</i> , 1973, 6, 238-245.	15.6	10
50	Theoretical Adsorption Studies of HCN and HNC on Ni(111). <i>The Journal of Physical Chemistry</i> , 1996, 100, 5090-5097.	2.9	10
51	Theoretical treatment of excited electronic states of adsorbates on metals: Electron attachment to CO <sub>2</sub> adsorbed on Pt(111). <i>Surface Science</i> , 2007, 601, 3755-3759.	1.9	9
52	Helium Difluoride. <i>Journal of the American Chemical Society</i> , 1965, 87, 3769-3771.	13.7	8
53	Integration of Plasma-Assisted and Rapid Thermal Processing for Low-Thermal Budget Preparation of Ultra-Thin Dielectrics for Stacked-Gate Device Structures. <i>Japanese Journal of Applied Physics</i> , 1994, 33, 7061-7070.	1.5	8
54	Bonding of carbon to nickel surfaces: effects of subsurface Na, H and C. <i>Applied Surface Science</i> , 1994, 75, 12-20.	6.1	8

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55	Theoretical Study of the CH <sub>2</sub> + O Photodissociation of Formaldehyde Adsorbed on the Ag(111) Surface. Journal of Physical Chemistry B, 2005, 109, 18070-18080.	2.6	8
56	Adsorption of copper on a $\gamma$ -alumina support. Surface Science, 2016, 651, 22-27.	1.9	8
57	Understanding the electrospray ionization response factors of per- and poly-fluoroalkyl substances (PFAS). Analytical and Bioanalytical Chemistry, 2022, 414, 1227-1234.	3.7	8
58	Quantum Catalysis: The Modeling of Catalytic Transition States. ACS Symposium Series, 1999, , 2-17.	0.5	7
59	Band offset energies in zirconium silicate Si alloys. Applied Surface Science, 2003, 216, 215-222.	6.1	7
60	Photoinduced Dissociation of Water and Transport of Hydrogen between Silver Clusters. Journal of Physical Chemistry A, 2008, 112, 6358-6363.	2.5	7
61	Theoretical Study of the Molecular and Electronic Structures of TiO <sub>4</sub> H <sub>4</sub> , Ti <sub>2</sub> O <sub>7</sub> H <sub>6</sub> , and Ti <sub>2</sub> O <sub>6</sub> H <sub>4</sub> . Journal of Physical Chemistry C, 2011, 115, 1635-1642.	3.1	7
62	Iterative natural orbitals for configuration interaction using perturbation theory. Theoretica Chimica Acta, 1977, 44, 305-313.	0.8	6
63	Ab initio evaluation of the Born correction, Born couplings, and higher derivative matrix elements with Gaussian-type orbitals. Journal of Chemical Physics, 1988, 88, 7662-7670.	3.0	6
64	Effects of subsurface Na, H and C on the bonding of carbon to nickel surfaces. Surface Science, 1993, 294, L945-L951.	1.9	6
65	Reaction of CH <sub>4</sub> with substitutional Fe/Ni(111). Surface Science, 1993, 289, 30-38.	1.9	6
66	Adsorption Energetics of NO and CO on Pt(111). Journal of Cluster Science, 1999, 10, 581-590.	3.3	6
67	Prediction of many-electron wavefunctions using atomic potentials. Journal of Chemical Physics, 2017, 146, 194109.	3.0	6
68	Reaction of Methane with Nickel [111] Surface. ACS Symposium Series, 1989, , 140-152.	0.5	5
69	Reaction of CH <sub>4</sub> and CH <sub>3</sub> F with Si(111). Journal of Electron Spectroscopy and Related Phenomena, 1994, 69, 23-29.	1.7	5
70	Theoretical treatment of excited electronic states of adsorbates on metals: Electron attachment to CO <sub>2</sub> adsorbed on K-modified Pt(111). Surface Science, 2008, 602, 834-842.	1.9	5
71	Photoinduced dissociation of water adsorbed on a Ag cluster. Computational and Theoretical Chemistry, 2009, 903, 28-33.	1.5	4
72	Configuration interaction study of the ground and excited states of TiO <sub>2</sub> ring structures. Journal of Chemical Physics, 2011, 134, 114701.	3.0	4

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73	Electronic structure and spectra of $(\text{Cu}_{2}\text{O})_{n}\text{H}_{2}\text{O}$ complexes. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 428-433.	2.8	4
74	Electron correlation by polarization of interacting densities. <i>Journal of Chemical Physics</i> , 2017, 146, 064113.	3.0	4
75	Prediction of many-electron wavefunctions using atomic potentials: extended basis sets and molecular dissociation. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 21541-21548.	2.8	4
76	Prediction of many-electron wavefunctions using atomic potentials: Refinements and extensions to transition metals and large systems. <i>Journal of Chemical Physics</i> , 2019, 150, 034107.	3.0	4
77	The Conceptual Dilemma of the One-Electron Picture in Describing the Uniaxial Magnetism at Linear Coordination Sites. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 2630-2634.	2.0	3
78	Materials and Processes for High k Gate Stacks: Results from the FEP Transition Center. <i>ECS Transactions</i> , 2006, 3, 389-415.	0.5	2
79	Effects of subsurface Na, H and C on $\text{CH}_3$ adsorption on Ni(111). <i>Surface Science Letters</i> , 1992, 277, L95-L99.	0.1	1
80	A molecular orbital model for the electronic structure of transition metal atoms in silicate and aluminate alloys. <i>Applied Surface Science</i> , 2002, 190, 48-55.	6.1	1
81	Theoretical Study of the Photoinduced $\text{C}\text{--}\text{H}$ Bond Cleavage in Formaldehyde Adsorbed on the Ag(111) Surface. <i>Journal of Physical Chemistry C</i> , 2007, 111, 9914-9918.	3.1	1
82	Estimates of electron correlation based on density expansions. <i>Journal of Chemical Physics</i> , 2020, 153, 244103.	3.0	1
83	Influence of surface impurity on impact response of lattices. <i>Journal of Applied Physics</i> , 1990, 67, 1397-1407.	2.5	0
84	Effects of subsurface Na, H and C on the bonding of carbon to nickel surfaces. <i>Surface Science Letters</i> , 1993, 294, L945-L951.	0.1	0
85	Band-Edge Electronic States, and Pre-Existing Defects in Remote Plasma Deposited (RPD) $\text{GeO}_2$ and $\text{SiO}_2$ . , 2012, , .		0
86	Chemical bonding and electronic structure of high- $\kappa$ transition metal dielectrics: applications to interfacial band offset energies and electronically active defects. , 0, , .		0