

Julius Jellinek

List of Publications by Year in descending order

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68
papers

7,009
citations

136950

32
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102487

66
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73
all docs

73
docs citations

73
times ranked

6905
citing authors

#	ARTICLE	IF	CITATIONS
1	Nanoalloys: From Theory to Applications of Alloy Clusters and Nanoparticles. Chemical Reviews, 2008, 108, 845-910.	47.7	3,234
2	Solid-liquid phase changes in simulated isoenergetic Ar ₁₃ . Journal of Chemical Physics, 1986, 84, 2783-2794.	3.0	501
3	Rare gas clusters: Solids, liquids, slush, and magic numbers. Journal of Chemical Physics, 1987, 87, 545-554.	3.0	298
4	Melting of clusters and melting. Physical Review A, 1984, 30, 919-931.	2.5	225
5	Melting and freezing in isothermal Ar ₁₃ clusters. Journal of Chemical Physics, 1987, 86, 6456-6464. Static polarizabilities and optical absorption spectra of gold clusters ($\langle \alpha \rangle$). Journal of Chemical Physics, 1987, 86, 5621-5624.	3.0	197
6		3.2	161
7	Capping Ligands as Selectivity Switchers in Hydrogenation Reactions. Nano Letters, 2012, 12, 5382-5388.	9.1	146
8	Structure and Magnetism of VnBzn+1 Sandwich Clusters. Journal of the American Chemical Society, 2005, 127, 2812-2813.	13.7	145
9	Magnesium Clusters: Structural and Electronic Properties and the Size-Induced Nonmetal-to-Metal Transition. Journal of Physical Chemistry A, 2002, 106, 10919-10925.	2.5	134
10	Solid-Liquid Phase Behavior in Microclusters. Advances in Chemical Physics, 2007, , 75-138.	0.3	128
11	Separation of the Energy of Overall Rotation in AnyN-Body System. Physical Review Letters, 1989, 62, 241-244.	7.8	113
12	Nanoalloys: tuning properties and characteristics through size and composition. Faraday Discussions, 2008, 138, 11.	3.2	103
13	Hollow Cages versus Space-Filling Structures for Medium-Sized Gold Clusters: The Spherical Aromaticity of the Au ₅₀ Cage. Journal of Physical Chemistry A, 2005, 109, 9265-9269.	2.5	101
14	Structure and shape variations in intermediate-size copper clusters. Journal of Chemical Physics, 2006, 124, 024308.	3.0	100
15	Electron Binding Energies of Anionic Magnesium Clusters and the Nonmetal-to-Metal Transition. Physical Review Letters, 2002, 89, 213402.	7.8	89
16	Unequal freezing and melting temperatures for clusters. Chemical Physics Letters, 1984, 107, 227-230.	2.6	86
17	Fragmentation of atomic clusters: A theoretical study. Physical Review A, 1994, 50, 1445-1458.	2.5	76
18	Structural Evolution of Anionic Silicon Clusters SiN(20-45). Journal of Physical Chemistry A, 2006, 110, 908-912.	2.5	75

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19	Quantum mechanical treatment of the $F+H_2^+\rightarrow HF+H$ reaction. Journal of Chemical Physics, 1983, 78, 2962-2977.	3.0	63
20	Aqueous Phase Glycerol Reforming by PtMo Bimetallic Nano-Particle Catalyst: Product Selectivity and Structural Characterization. Topics in Catalysis, 2012, 55, 53-69.	2.8	62
21	Gold-Coated Transition-Metal Anion [Mn ¹³ @Au ₂₀]-with Ultrahigh Magnetic Moment. Journal of the American Chemical Society, 2007, 129, 4110-4111.	13.7	58
22	Electronic and optical excitations in Ag _n . Physical Review B, 2009, 79, .	3.2	56
23	Supported Single-Site Ti(IV) on a Metal-Organic Framework for the Hydroboration of Carbonyl Compounds. Organometallics, 2017, 36, 3921-3930.	2.3	50
24	First-principles absorption spectra of Cu _n . Physical Review B, 2009, 79, .	3.2	45
25	Infrared Spectra of VnBzn+1 Sandwich Clusters: A Theoretical Study of Size Evolution. Journal of Physical Chemistry A, 2005, 109, 10180-10182.	2.5	44
26	Dipole polarizabilities of medium-sized gold clusters. Physical Review A, 2006, 74, .	2.5	41
27	Structural and electronic properties of small beryllium clusters: A theoretical study. Journal of Chemical Physics, 2004, 121, 7243-7252.	3.0	40
28	Structural, Electronic, and Optical Properties of Noble Metal Clusters from First Principles. Journal of Cluster Science, 2006, 17, 609-626.	3.3	39
29	Generalization of Nosé-Hoover isothermal molecular dynamics. Physical Review A, 1988, 38, 3069-3072.	2.5	37
30	Quantum-Mechanical State-to-State Differential Cross Sections for the Reaction $F + H_2^+ \rightarrow H + HF$. Physical Review Letters, 1981, 47, 1588-1592.	7.8	35
31	H_2 Reactions on Palladium Clusters. Journal of Physical Chemistry A, 2013, 117, 10407-10415.	2.5	35
32	Converting Kohn-Sham eigenenergies into electron binding energies. Journal of Chemical Physics, 2003, 118, 7783-7796.	3.0	32
33	Aqueous Phase Glycerol Reforming with Pt and PtMo Bimetallic Nanoparticle Catalysts: The Role of the Mo Promoter. Topics in Catalysis, 2013, 56, 1814-1828.	2.8	32
34	Mn ⁿ clusters: Size-induced transition to half metallicity. Physical Review B, 2006, 74, .	3.2	31
35	First-principles isomer-specific absorption spectra of Ag ₁₁ . Physical Review B, 2007, 75, .	3.2	28
36	Theoretical Investigation of Adsorption of Molecular Oxygen on Small Copper Clusters. Journal of Physical Chemistry A, 2011, 115, 8705-8712.	2.5	28

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37	Infinite order sudden approximation for reactive scattering within classical mechanics. I. Theory. Journal of Chemical Physics, 1982, 76, 4883-4892.	3.0	27
38	An adiabatic analysis of the reactive infinite order sudden approximation. Journal of Chemical Physics, 1983, 78, 3014-3020.	3.0	27
39	The shapes of first-stage sinters. Journal of Applied Physics, 1989, 65, 3219-3225.	2.5	27
40	Ab initio Monte Carlo: application to Li ₈ . Chemical Physics Letters, 1998, 288, 705-713.	2.6	24
41	Generalization of Nosé's isothermal molecular dynamics: Necessary and sufficient conditions of dynamical simulations of statistical ensembles. Physical Review A, 1989, 40, 2816-2818.	2.5	20
42	Br ₂ (X) Microsolvation in Helium Clusters: Effect of the Interaction on the Quantum Solvent Density Distribution. ChemPhysChem, 2005, 6, 1348-1356.	2.1	19
43	REACTION DYNAMICS OF Ni _n (n = 19 and 20) WITH D ₂ : DEPENDENCE ON CLUSTER SIZE, TEMPERATURE AND INITIAL ROVIBRATIONAL STATES OF THE MOLECULE. International Journal of Modern Physics C, 2005, 16, 295-308.	1.7	18
44	A classical reactive study within the infinite order sudden approximation: integral cross sections for	2.6	17
45	H ₂ Saturation on Palladium Clusters. Journal of Physical Chemistry A, 2015, 119, 3594-3603.	2.5	17
46	Investigating the metallic behavior of Na clusters using site-specific polarizabilities. Physical Review B, 2014, 89, .	3.2	16
47	Trajectory studies within the framework of the infinite order sudden approximation for the F+H ₂ →HF+H reaction. Journal of Chemical Physics, 1983, 78, 4494-4501.	3.0	13
48	Space-time properties of Gram-Schmidt vectors in classical Hamiltonian evolution. Physical Review E, 2009, 80, 066205.	2.1	11
49	Si clusters are more metallic than bulk Si. Journal of Chemical Physics, 2016, 145, 244302.	3.0	11
50	Morphology Tailoring of Pt Nanocatalysts for the Oxygen Reduction Reaction: The Paradigm of Pt ₁₃ . ChemNanoMat, 2015, 1, 482-488.	2.8	10
51	Theoretical investigations of the interaction of silver trimer with ethylene molecule. Chemical Physics Letters, 2001, 345, 312-318.	2.6	9
52	Reactive scattering calculations for ⁸⁷ Rb+ ⁸⁷ RbHe→Rb ₂ (3 ¹ Σ ⁺ _u ,v)+He from ultralow to intermediate energies. Journal of Chemical Physics, 2015, 142, 164304.	3.0	8
53	On the classical mechanical reactive infinite order sudden approximation. Chemical Physics Letters, 1985, 114, 210-216.	2.6	6
54	Thermal behavior of a 13-molecule hydrogen cluster under pressure. Journal of Chemical Physics, 2010, 132, 124505.	3.0	6

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55	Theoretical Analysis of Photoelectron Spectra of Pure and Mixed Metal Clusters: Disentangling Size, Structure, and Composition Effects. <i>Journal of Physical Chemistry C</i> , 2017, 121, 16665-16672.	3.1	6
56	Electron Binding Energy Spectra of Al _n Mo ⁺ Clusters: Measurements, Calculations, and Theoretical Analysis. <i>Journal of Physical Chemistry C</i> , 2019, 123, 7810-7817.	3.1	5
57	Site-specific polarizabilities as predictors of favorable adsorption sites on Nan clusters. <i>Chemical Physics Letters</i> , 2011, 503, 80-85.	2.6	4
58	Anharmonic densities of states: A general dynamics-based solution. <i>Journal of Chemical Physics</i> , 2016, 144, 214103.	3.0	4
59	Characterizing Metal Coordination Environments in Porous Organic Polymers: A Joint Density Functional Theory and Experimental Infrared Spectroscopy Study. <i>Chemistry - A European Journal</i> , 2013, 19, 13646-13651.	3.3	3
60	Computational studies of structural, energetic, and electronic properties of pure Pt and Mo and mixed Pt/Mo clusters: Comparative analysis of characteristics and trends. <i>Journal of Chemical Physics</i> , 2022, 157, .	3.0	3
61	Electron Binding Energy Spectra of Al _n Pt ⁺ Clusters – A Combined Experimental and Computational Study. <i>Journal of Physical Chemistry A</i> , 0, .	2.5	3
62	Kinematics of the two-angle-dependent reactive infinite-order sudden approximation. <i>Journal of Mathematical Physics</i> , 1985, 26, 1397-1403.	1.1	2
63	Pressure-Induced Metallization of Li ⁺ -Doped Hydrogen Clusters. <i>Journal of Physical Chemistry A</i> , 2013, 117, 5642-5649.	2.5	2
64	Universality in size-driven evolution towards bulk polarizability of metals. <i>Nanoscale</i> , 2018, 10, 17534-17539.	5.6	2
65	Range effects of the Coulombic forces on structures, thermodynamic properties and potential energy landscapes: (KCl) ₃₂ and related systems. <i>Chemical Physics</i> , 2012, 399, 281-289.	1.9	1
66	D2 +Ni _n (T), n=7 and 9, Collision System. <i>Mathematical and Computational Applications</i> , 1999, 4, 61-67.	1.3	0
67	Structural Forms and Energies of Ni _n , n=12-14, Clusters. <i>Mathematical and Computational Applications</i> , 1999, 4, 75-81.	1.3	0
68	Fragmentation of a Non-Rotating Ni ₁₉ Cluster: A Molecular Dynamics Study. <i>Mathematical and Computational Applications</i> , 1999, 4, 99-106.	1.3	0