Julius Jellinek

List of Publications by Year
in descending order

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68	7,009	136950	102487
papers	citations	32 h-index	66 g-index

73	73	73	6905
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Computational studies of structural, energetic, and electronic properties of pure Pt and Mo and mixed Pt/Mo clusters: Comparative analysis of characteristics and trends. Journal of Chemical Physics, 2022, 157, .	3.0	3
2	Electron Binding Energy Spectra of Al_nMo^{â€“} Clusters: Measurements, Calculations, and Theoretical Analysis. Journal of Physical Chemistry C, 2019, 123, 7810-7817.	3.1	5
3	Universality in size-driven evolution towards bulk polarizability of metals. Nanoscale, 2018, 10, 17534-17539.	5.6	2
4	Supported Single-Site Ti(IV) on a Metalâ€“Organic Framework for the Hydroboration of Carbonyl Compounds. Organometallics, 2017, 36, 3921-3930.	2.3	50
5	Theoretical Analysis of Photoelectron Spectra of Pure and Mixed Metal Clusters: Disentangling Size, Structure, and Composition Effects. Journal of Physical Chemistry C, 2017, 121, 16665-16672.	3.1	6
6	Anharmonic densities of states: A general dynamics-based solution. Journal of Chemical Physics, 2016, 144, 214103.	3.0	4
7	Si clusters are more metallic than bulk Si. Journal of Chemical Physics, 2016, 145, 244302.	3.0	11
8	Morphology Tailoring of Pt Nanocatalysts for the Oxygen Reduction Reaction: The Paradigm of Pt₁₃. ChemNanoMat, 2015, 1, 482-488.	2.8	10
9	H₂ Saturation on Palladium Clusters. Journal of Physical Chemistry A, 2015, 119, 3594-3603.	2.5	17
10	Reactive scattering calculations for 87Rb+87RbHeâ†'Rb2(3Î£u+,v)+He from ultralow to intermediate energies. Journal of Chemical Physics, 2015, 142, 164304.	3.0	8
11	Investigating the metallic behavior of Na clusters using site-specific polarizabilities. Physical Review B, 2014, 89, .	3.2	16
12	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
13	H₂ Reactions on Palladium Clusters. Journal of Physical Chemistry A, 2013, 117, 10407-10415.	2.5	35
14	Pressure-Induced Metallization of Li⁺-Doped Hydrogen Clusters. Journal of Physical Chemistry A, 2013, 117, 5642-5649.	2.5	2
15	Characterizing Metal Coordination Environments in Porous Organic Polymers: A Joint Density Functional Theory and Experimental Infrared Spectroscopy Study. Chemistry - A European Journal, 2013, 19, 13646-13651.	3.3	3
16	Capping Ligands as Selectivity Switchers in Hydrogenation Reactions. Nano Letters, 2012, 12, 5382-5388.	9.1	146
17	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
18	Range effects of the Coulombic forces on structures, thermodynamic properties and potential energy landscapes: (KCl)32 and related systems. Chemical Physics, 2012, 399, 281-289.	1.9	1

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19	Theoretical Investigation of Adsorption of Molecular Oxygen on Small Copper Clusters. Journal of Physical Chemistry A, 2011, 115, 8705-8712.	2.5	28
20	Site-specific polarizabilities as predictors of favorable adsorption sites on Nan clusters. Chemical Physics Letters, 2011, 503, 80-85.	2.6	4
21	First-principles absorption spectra of Cu<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mi>n</mml:mi></mml:mrow></mml:msub></mml:mrow></mml:math>(<mml:math) Tj ETQq1 1 0.784314 rgBT /O	3.2	45
22	Thermal behavior of a 13-molecule hydrogen cluster under pressure. Journal of Chemical Physics, 2010, 132, 124505.	3.0	6
23	Space-time properties of Gram-Schmidt vectors in classical Hamiltonian evolution. Physical Review E, 2009, 80, 066205.	2.1	11
24	Electronic and optical excitations in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ag</mml:mtext></mml:mrow><mml:mi>n</mml:mi></mml:msub><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:mi>n</mml:mi><mml:mo>=</mml:mo><mml:mn> Physical Review B, 2009, 79, .	3.2	56
25	Nanoalloys:â€‰ From Theory to Applications of Alloy Clusters and Nanoparticles. Chemical Reviews, 2008, 108, 845-910.	47.7	3,234
26	Nanoalloys: tuning properties and characteristics through size and composition. Faraday Discussions, 2008, 138, 11.	3.2	103
27	First-principles isomer-specific absorption spectra ofAg11. Physical Review B, 2007, 75, .	3.2	28
28	Solid-Liquid Phase Behavior in Microclusters. Advances in Chemical Physics, 2007, , 75-138.	0.3	128
29	Static polarizabilities and optical absorption spectra of gold clusters (<mml:math) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 362 Td	3.2	161
30	Gold-Coated Transition-Metal Anion [Mn13@Au20]-with Ultrahigh Magnetic Moment. Journal of the American Chemical Society, 2007, 129, 4110-4111.	13.7	58
31	Structure and shape variations in intermediate-size copper clusters. Journal of Chemical Physics, 2006, 124, 024308.	3.0	100
32	Structural Evolution of Anionic Silicon Clusters SiN(20 â‰¤Nâ‰¤ 45). Journal of Physical Chemistry A, 2006, 110, 908-912.	2.5	75
33	Structural, Electronic, and Optical Properties of Noble Metal Clusters from First Principles. Journal of Cluster Science, 2006, 17, 609-626.	3.3	39
34	Mnnâ^'clusters: Size-induced transition to half metallicity. Physical Review B, 2006, 74, .	3.2	31
35	Dipole polarizabilities of medium-sized gold clusters. Physical Review A, 2006, 74, .	2.5	41
36	Br2(X) Microsolvation in Helium Clusters: Effect of the Interaction on the Quantum Solvent Density Distribution. ChemPhysChem, 2005, 6, 1348-1356.	2.1	19

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37	REACTION DYNAMICS OF Nin (n =19 and 20) WITH D2: 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
38	Hollow Cages versus Space-Filling Structures for Medium-Sized Gold Clusters:â€‰ The Spherical Aromaticity of the Au50 Cage. Journal of Physical Chemistry A, 2005, 109, 9265-9269.	2.5	101
39	Infrared Spectra of VnBzn+1 Sandwich Clusters:â€‰ A Theoretical Study of Size Evolution. Journal of Physical Chemistry A, 2005, 109, 10180-10182.	2.5	44
40	Structure and Magnetism of VnBzn+1Sandwich Clusters. Journal of the American Chemical Society, 2005, 127, 2812-2813.	13.7	145
41	Structural and electronic properties of small beryllium clusters: A theoretical study. Journal of Chemical Physics, 2004, 121, 7243-7252.	3.0	40
42	Converting Kohnâ€“Sham eigenenergies into electron binding energies. Journal of Chemical Physics, 2003, 118, 7783-7796.	3.0	32
43	Magnesium Clusters:Â Structural and Electronic Properties and the Size-Induced Nonmetal-to-Metal Transitionâ€. Journal of Physical Chemistry A, 2002, 106, 10919-10925.	2.5	134
44	Electron Binding Energies of Anionic Magnesium Clusters and the Nonmetal-to-Metal Transition. Physical Review Letters, 2002, 89, 213402.	7.8	89
45	Theoretical investigations of the interaction of silver trimer with ethylene molecule. Chemical Physics Letters, 2001, 345, 312-318.	2.6	9
46	D2 +Nin(T), n=7 and 9, Collision System. Mathematical and Computational Applications, 1999, 4, 61-67.	1.3	0
47	Structural Forms and Energies of Nin, n=12-14, Clusters. Mathematical and Computational Applications, 1999, 4, 75-81.	1.3	0
48	Fragmentation of a Non-Rotating Ni19 Cluster: A Molecular Dynamics Study. Mathematical and Computational Applications, 1999, 4, 99-106.	1.3	0
49	Ab initio Monte Carlo: application to Li8. Chemical Physics Letters, 1998, 288, 705-713.	2.6	24
50	Fragmentation of atomic clusters: A theoretical study. Physical Review A, 1994, 50, 1445-1458.	2.5	76
51	Separation of the Energy of Overall Rotation in AnyN-Body System. Physical Review Letters, 1989, 62, 241-244.	7.8	113
52	Generalization of NosÃ©â€™s isothermal molecular dynamics: Necessary and sufficient conditions of dynamical simulations of statistical ensembles. Physical Review A, 1989, 40, 2816-2818.	2.5	20
53	The shapes of firstâ€stage sinters. Journal of Applied Physics, 1989, 65, 3219-3225.	2.5	27
54	Generalization of NosÃ©â€™s isothermal molecular dynamics. Physical Review A, 1988, 38, 3069-3072.	2.5	37

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55	Melting and freezing in isothermal Ar13 clusters. Journal of Chemical Physics, 1987, 86, 6456-6464.	3.0	197
56	Rare gas clusters: Solids, liquids, slush, and magic numbers. Journal of Chemical Physics, 1987, 87, 545-554.	3.0	298
57	Solidâ€“liquid phase changes in simulated isoenergetic Ar13. Journal of Chemical Physics, 1986, 84, 2783-2794.	3.0	501
58	Kinematics of the twoâ€angleâ€dependent reactive infiniteâ€order sudden approximation. Journal of Mathematical Physics, 1985, 26, 1397-1403.	1.1	2
59	On the classical mechanical reactive infinite order sudden approximation. Chemical Physics Letters, 1985, 114, 210-216.	2.6	6
60	Unequal freezing and melting temperatures for clusters. Chemical Physics Letters, 1984, 107, 227-230.	2.6	86
61	Melting of clusters and melting. Physical Review A, 1984, 30, 919-931.	2.5	225
62	Quantum mechanical treatment of the F+H2â†'HF+H reaction. Journal of Chemical Physics, 1983, 78, 2962-2977.	3.0	63
63	An adiabatic analysis of the reactive infinite order sudden approximation. Journal of Chemical Physics, 1983, 78, 3014-3020.	3.0	27
64	Trajectory studies within the framework of the infinite order sudden approximation for the F+H2â†'HF+H reaction. Journal of Chemical Physics, 1983, 78, 4494-4501.	3.0	13
65	Infinite order sudden approximation for reactive scattering within classical mechanics. I. Theory. Journal of Chemical Physics, 1982, 76, 4883-4892.	3.0	27
66	A classical reactive study within the infinite order sudden approximation: integral cross sections for	2.6	17
67	Quantum-Mechanical State-to-State Differential Cross Sections for the Reaction F +H2â†' H + HF. Physical Review Letters, 1981, 47, 1588-1592.	7.8	35
68	Electron Binding Energy Spectra of Al_nPt^{â€“} Clustersâ”€A Combined Experimental and Computational Study. Journal of Physical Chemistry A, 0, , .	2.5	3