Julio A Alonso

List of Publications by Year
in descending order

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406 papers	10,586 citations	41344 49 h-index	51608 86 g-index
414 all docs	414 docs citations	414 times ranked	7205 citing authors

#	Article	IF	Citations
1	Palladium clusters, free and supported on surfaces, and their applications in hydrogen storage. Physical Chemistry Chemical Physics, 2022, 24, 2729-2751.	2.8	9
2	Catalytic activity of Coâ€“Ag nanoalloys to dissociate molecular hydrogen. New insights on the chemical environment. International Journal of Hydrogen Energy, 2022, 47, 19038-19050.	7.1	3
3	Concentration asymmetry and carbon enrichment in titanium carbide and silicon carbide clusters. Physical Review A, 2022, 105, .	2.5	2
4	Infrared spectra and structures of C60Rhn+ complexes. Carbon, 2022, 197, 535-543.	10.3	7
5	Effects of van der Waals interactions on the structure and stability of Cu8-xPdx (x = 0, 4, 8) cluster isomers. Materials Today Communications, 2021, 26, 102024.	1.9	9
6	Interaction of hydrogen with palladiumâ€“copper nanoalloys. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	7
7	Theoretical Study of the Diels-Alder Dimerization of C30H10. ECS Meeting Abstracts, 2021, MA2021-01, 645-645.	0.0	0
8	Adsorption of transition metal clusters on Boron-graphdiyne. Applied Surface Science, 2021, 548, 149270.	6.1	4
9	C60Con complexes as hydrogen adsorbing materials. International Journal of Hydrogen Energy, 2021, 46, 20594-20606.	7.1	7
10	Absence of spillover of hydrogen adsorbed on small palladium clusters anchored to graphene vacancies. Applied Surface Science, 2021, 559, 149835.	6.1	17
11	Ultra-stable nanofluid containing Functionalized-Carbon Dots for heat transfer enhancement in Water/Ethylene glycol systems: Experimental and DFT studies. Energy Reports, 2021, 7, 4222-4234.	5.1	15
12	Hydrogen Interaction with Tungsten Disulfide Nanostructures. , 2021, , .		0
13	Nanoalloys of Metals Which Do Not Form Bulk Alloys: The Case of Agâ€“Co. Journal of Physical Chemistry A, 2020, 124, 6468-6477.	2.5	12
14	Cathodoluminescence in single and multiwall WS2 nanotubes: Evidence for quantum confinement and strain effect. Applied Physics Reviews, 2020, 7, .	11.3	15
15	Dimerization of pentacyclopentacorannulene C30H10 as a strategy to produce C60H20 as a precursor for C60. RSC Advances, 2020, 10, 3689-3693.	3.6	3
16	Reactivity of Cobaltâ€Fullerene Complexes towards Deuterium. ChemPhysChem, 2020, 21, 1012-1018.	2.1	8
17	Interaction of Hydrogen with Graphitic Surfaces, Clean and Doped with Metal Clusters. , 2020, , 545-566.		0
18	Dynamics of Cluster Isomerization Induced by Hydrogen Adsorption. Journal of Physical Chemistry C, 2019, 123, 15236-15243.	3.1	12

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19	Hydrogen quenches the size effects in carbon clusters. Physical Chemistry Chemical Physics, 2019, 21, 10402-10410.	2.8	3
20	Bimetallic Alâ€“Sn clusters: mixing at the nanoscale. Physical Chemistry Chemical Physics, 2019, 21, 22919-22929.	2.8	8
21	H₂ Adsorption on Cu_{4-x}M_x (M = Au, Pt; x = 0â€“4) Clusters: Similarities and Differences As Predicted by Density Functional Theory. Journal of Physical Chemistry C, 2019, 123, 30768-30780.	3.1	13
22	Ab initio studies of ethanol dehydrogenation at binary AuPd nanocatalysts. Molecular Catalysis, 2018, 449, 8-13.	2.0	14
23	Modelling of adsorption and intercalation of hydrogen on/into tungsten disulphide multilayers and multiwall nanotubes. Physical Chemistry Chemical Physics, 2018, 20, 12061-12074.	2.8	6
24	An improved descriptor of cluster stability: application to small carbon clusters. Physical Chemistry Chemical Physics, 2018, 20, 27368-27374.	2.8	8
25	Theoretical study of the adsorption of hydrogen on cobalt clusters. Physical Chemistry Chemical Physics, 2018, 20, 21163-21176.	2.8	19
26	Interaction of Hydrogen with Graphitic Surfaces, Clean and Doped with Metal Clusters. , 2018, , 1-22.		0
27	Competition between Palladium Clusters and Hydrogen to Saturate Graphene Vacancies. Journal of Physical Chemistry C, 2017, 121, 10843-10850.	3.1	21
28	Steric and chemical effects on the hydrogen adsorption and dissociation on free and grapheneâ€“supported palladium clusters. Computational and Theoretical Chemistry, 2017, 1107, 23-29.	2.5	25
29	Hydrogen Chemical Configuration and Thermal Stability in Tungsten Disulfide Nanoparticles Exposed to Hydrogen Plasma. Journal of Physical Chemistry C, 2017, 121, 11747-11756.	3.1	6
30	Interaction of aromatic molecules with small gold clusters. Chemical Physics Letters, 2017, 684, 91-96.	2.6	10
31	Searching for DFT-based methods that include dispersion interactions to calculate the physisorption of H2 on benzene and graphene. Journal of Chemical Physics, 2017, 146, 214104.	3.0	30
32	Manipulating the Magnetic Moment of Palladium Clusters by Adsorption and Dissociation of Molecular Hydrogen. Journal of Physical Chemistry C, 2017, 121, 20756-20762.	3.1	12
33	Adsorption and growth of palladium clusters on graphdiyne. Physical Chemistry Chemical Physics, 2017, 19, 19094-19102.	2.8	40
34	The Storage of Hydrogen in Nanoporous Carbons. Journal of the Mexican Chemical Society, 2017, 56, .	0.6	2
35	The Diels-Alder Cycloaddition Reaction of Substituted Hemifullerenes with 1,3-Butadiene: Effect of Electron-Donating and Electron-Withdrawing Substituents. Molecules, 2016, 21, 200.	3.8	7
36	Controlling the Adsorption of Carbon Monoxide on Platinum Clusters by Dopantâ€Induced Electronic Structure Modification. Angewandte Chemie - International Edition, 2016, 55, 11059-11063.	13.8	55

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37	Is Spillover Relevant for Hydrogen Adsorption and Storage in Porous Carbons Doped with Palladium Nanoparticles?. Journal of Physical Chemistry C, 2016, 120, 17357-17364.	3.1	51
38	Controlling the Adsorption of Carbon Monoxide on Platinum Clusters by Dopantâ€Induced Electronic Structure Modification. Angewandte Chemie, 2016, 128, 11225-11229.	2.0	25
39	Interaction of hydrogen with palladium clusters deposited on graphene. AIP Conference Proceedings, 2015, , .	0.4	0
40	Elimination vs Substitution Reaction. A Dichotomy between BrÃ¸nstedâ€“Lowry and Lewis Basicity. Organic Letters, 2015, 17, 767-769.	4.6	2
41	The diatomic dication SiC2+ in the gas phase. Chemical Physics, 2015, 455, 41-47.	1.9	1
42	Competition between molecular and dissociative adsorption of hydrogen on palladium clusters deposited on defective graphene. RSC Advances, 2015, 5, 47945-47953.	3.6	45
43	From graphene oxide to pristine graphene: revealing the inner workings of the full structural restoration. Nanoscale, 2015, 7, 2374-2390.	5.6	95
44	Nanostructure Oxide, Metal Oxide and Composite Cylindrical Shapes For Energy and Electromagnetic Spectrum Uses: First Principles Structural, Electronic, and Transport Characterization of SiO2 NanoWires, RuO2 NanoTubes, and SiO2/RuO2 NanoCables. , 2014, , .		0
45	Ab initio studies of propene epoxidation on oxidized silver surfaces. Physical Chemistry Chemical Physics, 2014, 16, 26546-26552.	2.8	17
46	Metallicity enhancement in coreâ€“shell SiO2@RuO2nanowires. RSC Advances, 2014, 4, 34696-34700.	3.6	1
47	Palladium Clusters Anchored on Graphene Vacancies and Their Effect on the Reversible Adsorption of Hydrogen. Journal of Physical Chemistry C, 2014, 118, 5081-5090.	3.1	73
48	Tailoring structural and electronic properties of RuO2 nanotubes: a many-body approach and electronic transport. Physical Chemistry Chemical Physics, 2013, 15, 14715.	2.8	23
49	Protophilicity index and protofelicity equalization principle: new measures of BrÃ¸nsted-Lowry-Lewis acidâ€“base interactions. Journal of Molecular Modeling, 2013, 19, 3961-3967.	1.8	2
50	Simulation of hydrogen storage in porous carbons. Journal of Materials Research, 2013, 28, 589-604.	2.6	31
51	Evolution of the atomic structure and the magnetism of small oxygen clusters. Computational and Theoretical Chemistry, 2013, 1021, 215-221.	2.5	3
52	Semiempirical fine-tuning for Hartreeâ€“Fock ionization potentials of atomic ions with non-integral atomic number. Physics Letters, Section A: General, Atomic and Solid State Physics, 2013, 377, 2955-2958.	2.1	3
53	Transport coefficients in the strongly coupled liquid alkali metals. Physics Letters, Section A: General, Atomic and Solid State Physics, 2013, 377, 810-812.	2.1	1
54	Electronic and magnetic properties of Fe clusters inside finite zigzag single-wall carbon nanotubes. Physical Review B, 2013, 87, .	3.2	8

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55	Synthesis of fullerenes. Journal of Physical Organic Chemistry, 2013, 26, 526-539.	1.9	101
56	Comment on â€œThe diatomic dication CuZn2+ in the gas phaseâ€•[J. Chem. Phys. 135, 034306 (2011)]. Journal of Chemical Physics, 2013, 138, 077101.	3.0	0
57	Model for the Formation of Helium Bubbles in Palladium. Croatica Chemica Acta, 2013, 86, 425-429.	0.4	0
58	Growth of Fullerene Fragments Using the Diels-Alder Cycloaddition Reaction: First Step towards a C60 Synthesis by Dimerization. Molecules, 2013, 18, 2243-2254.	3.8	6
59	Temperature dependence of the liquid structure factor of dense monatomic fluids in the long wavelength limit in relation to thermal expansivity. Philosophical Magazine Letters, 2012, 92, 133-135.	1.2	1
60	Ornsteinâ€“Zernike direct correlation function from diffraction experiments in supercooled liquid silicon and in disordered cobalt. Physics and Chemistry of Liquids, 2012, 50, 131-136.	1.2	1
61	Adsorption and dissociation of molecular hydrogen on the edges of graphene nanoribbons. Journal of Nanoparticle Research, 2012, 14, 1.	1.9	15
62	First-Principles Structural and Electronic Characterization of Ordered SiO₂ Nanowires. Journal of Physical Chemistry C, 2012, 116, 18973-18982.	3.1	22
63	Density functional study of low-lying isomers of SiO4, GeO4 and CO4, and their relation to tetrahedral solid phases. European Physical Journal D, 2012, 66, 1.	1.3	0
64	Adsorption and Dissociation of Molecular Hydrogen on Palladium Clusters Supported on Graphene. Journal of Physical Chemistry C, 2012, 116, 21179-21189.	3.1	104
65	Scattering of a proton with the Li4 cluster: Non-adiabatic molecular dynamics description based on time-dependent density-functional theory. Chemical Physics, 2012, 399, 130-134.	1.9	40
66	Surfactant effect of sulfuric acid on the exfoliation of bilayer graphene. Physical Review B, 2011, 84, .	3.2	15
67	Simulated porosity and electronic structure of nanoporous carbons. Journal of Chemical Physics, 2011, 135, 104706.	3.0	37
68	Theoretical Study of the Structural Stability and the Electronic Properties of Al_mH_n Clusters. Journal of Computational and Theoretical Nanoscience, 2011, 8, 609-615.	0.4	0
69	Simulation of the hydrogen storage in nanoporous carbons with different pore shapes. International Journal of Hydrogen Energy, 2011, 36, 10748-10759.	7.1	65
70	Modeling of the functionalization of single-wall carbon nanotubes towards its solubilization in an aqueous medium. European Physical Journal D, 2011, 61, 381-388.	1.3	14
71	Size-dependent selectivity and activity of silver nanoclusters in the partial oxidation of propylene to propylene oxide and acrolein: A joint experimental and theoretical study. Catalysis Today, 2011, 160, 116-130.	4.4	115
72	The diatomic dication CuZn2+ in the gas phase. Journal of Chemical Physics, 2011, 135, 034306.	3.0	5

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73	Some properties of the structure factorS(q) in two-dimensional classical liquids near freezing. Physics and Chemistry of Liquids, 2010, 48, 409-413.	1.2	4
74	Lifetime of electronic excitations in metal nanoparticles. New Journal of Physics, 2010, 12, 053023.	2.9	16
75	Optical to ultraviolet spectra of sandwiches of benzene and transition metal atoms: Time dependent density functional theory and many-body calculations. Journal of Chemical Physics, 2010, 132, 044314.	3.0	40
76	Theoretical study of the transition from planar to three-dimensional structures of palladium clusters supported on graphene. Physical Review B, 2010, 81, .	3.2	122
77	Interaction of Surfactants Containing a Sulfuric Group with a (5,5) Carbon Nanotube. Journal of Physical Chemistry C, 2010, 114, 17249-17256.	3.1	11
78	High-pressure behaviour of crystalline silane compared with that for SnH4. Phase Transitions, 2009, 82, 247-250.	1.3	2
79	Fractal network dimension determining the relation between the strength of bulk metallic glasses and the glass transition temperature. Applied Physics Letters, 2009, 95, 021909.	3.3	5
80	Observation of Zr22+, Cd22+, Hf22+, W22+, and Pt22+ in the gas phase. Journal of Chemical Physics, 2009, 130, 144312.	3.0	13
81	Properties of glass-forming metallic liquids: when is there a hard-sphere-like behaviour?. Physics and Chemistry of Liquids, 2009, 47, 585-598.	1.2	1
82	Selective Propene Epoxidation on Immobilized Au_{6â€“10} Clusters: The Effect of Hydrogen and Water on Activity and Selectivity. Angewandte Chemie - International Edition, 2009, 48, 1467-1471.	13.8	246
83	New insights on the reaction mechanisms for CO oxidation on Au catalysts. Chemical Physics Letters, 2009, 468, 201-204.	2.6	18
84	Adsorption of Lithium on Finite Graphitic Clusters. Journal of Physical Chemistry C, 2009, 113, 939-941.	3.1	34
85	A Combined Experimental and Theoretical Investigation of Atomic-Scale Defects Produced on Graphite Surfaces by Dielectric Barrier Discharge Plasma Treatment. Journal of Physical Chemistry C, 2009, 113, 18719-18729.	3.1	12
86	Transcending Lindemann's predictions for the melting temperatures of metals and for the long-wavelength limit of their liquid structure factors. Philosophical Magazine Letters, 2009, 89, 300-305.	1.2	7
87	Half-metallic finite zigzag single-walled carbon nanotubes from first principles. Physical Review B, 2008, 78, .	3.2	42
88	Hydrogen storage capacities of nanoporous carbon calculated by density functional and MÃ¸ller-Plesset methods. Physical Review B, 2008, 78, .	3.2	49
89	Non-monotonic behaviour with concentration of the surface tension of certain binary liquid alloys. Physics and Chemistry of Liquids, 2008, 46, 522-526.	1.2	10
90	Interaction of narrow carbon nanotubes with nitronium tetrafluoroborate salts. Journal of Chemical Physics, 2008, 128, 214703.	3.0	6

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91	Electronic and atomic structure of the AlnHn+2 clusters. Journal of Chemical Physics, 2008, 129, 074306.	3.0	15
92	Shape of the hydrogen adsorption regions of MOF-5 and its impact on the hydrogen storage capacity. Physical Review B, 2008, 78, .	3.2	13
93	Mechanism of amorphisation in Cuâ€“Ru, a binary alloy with a positive heat of mixing. Physics and Chemistry of Liquids, 2008, 46, 669-675.	1.2	5
94	Hydrogen storage in pure and Li-doped carbon nanopores: Combined effects of concavity and doping. Journal of Chemical Physics, 2008, 128, 144704.	3.0	53
95	Interaction and concerted diffusion of lithium in a (5,5) carbon nanotube. Physical Review B, 2008, 78, .	3.2	58
96	Ionization potentials of neutral atoms and positive ions in the limit of large atomic number. Physical Review A, 2007, 75, .	2.5	7
97	Two-parameter partially correlated ground-state electron density of some light spherical atoms from Hartree-Fock theory with nonintegral nuclear charge. Physical Review A, 2007, 75, .	2.5	13
98	Stability of silicon-doped C60 dimers. Journal of Chemical Physics, 2007, 126, 044705.	3.0	13
99	Chemical Properties of Small Au Clusters:â€‰ An Analysis of the Local Site Reactivity. Journal of Physical Chemistry C, 2007, 111, 6668-6677.	3.1	72
100	The interaction of sulfuric acid with graphene and formation of adsorbed crystals. Nanotechnology, 2007, 18, 485705.	2.6	33
101	Theoretical study of the photoabsorption spectrum of small chromium clusters. Physical Review B, 2007, 76, .	3.2	12
102	Interaction of the Charged Deuterium Cluster D3+with Femtosecond Laser Pulsesâ€. Journal of Physical Chemistry C, 2007, 111, 17765-17772.	3.1	14
103	The optimum average nanopore size for hydrogen storage in carbon nanoporous materials. Carbon, 2007, 45, 2649-2658.	10.3	168
104	Theoretical study of molecular hydrogen clusters. European Physical Journal D, 2007, 43, 61-64.	1.3	25
105	Long-Range van der Waals Interactions in Density Functional Theory. Theoretical Chemistry Accounts, 2007, 117, 467-472.	1.4	24
106	Density functional calculations of hydrogen adsorption on boron nanotubes and boron sheets. Nanotechnology, 2006, 17, 778-785.	2.6	83
107	Density functional study of molecular hydrogen coverage on carbon nanotubes. Computational Materials Science, 2006, 35, 238-242.	3.0	54
108	Calculation of metastable free-energy diagrams and glass formation in the Mgâ€“Cuâ€“Y alloy and its boundary binaries using the Miedema model. Intermetallics, 2006, 14, 297-307.	3.9	34

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109	Buckling in boron sheets and nanotubes. Physica Status Solidi (A) Applications and Materials Science, 2006, 203, 1105-1110.	1.8	22
110	Optical Absorption Spectra of V⁺₄ Isomers: One Example of First-Principles Theoretical Spectroscopy with Time-Dependent Density Functional Theory. Journal of Computational and Theoretical Nanoscience, 2006, 3, 761-766.	0.4	8
111	Photoabsorption spectra of Ti8C12 metallocarbohedrynes: Theoretical spectroscopy within time-dependent density functional theory. Journal of Chemical Physics, 2006, 125, 074311.	3.0	16
112	Structural corrections to Stokes-Einstein relation for liquid metals near freezing. Physical Review E, 2006, 73, 032201.	2.1	10
113	Electrostrictive deformations in small carbon clusters, hydrocarbon molecules, and carbon nanotubes. Physical Review A, 2006, 74, .	2.5	5
114	Optical Absorption Spectra of V⁺₄ Isomers: One Example of First-Principles Theoretical Spectroscopy with Time-Dependent Density Functional Theory. Journal of Computational and Theoretical Nanoscience, 2006, 3, 761-766.	0.4	8
115	Structural and thermal stability of narrow and short carbon nanotubes and nanostrips. Carbon, 2005, 43, 1371-1377.	10.3	38
116	Adsorption of hydrogen on normal and pentaheptite single wall carbon nanotubes. European Physical Journal D, 2005, 34, 279-282.	1.3	25
117	A density-functional study on the formation of Mo22+. Journal of Chemical Physics, 2005, 123, 134313.	3.0	6
118	BeB2nanostructures: A density functional study. Physical Review B, 2005, 72, .	3.2	6
119	Charging mechanism for the bond elongation observed in suspended chains of gold atoms. Physical Review B, 2005, 72, .	3.2	17
120	Fragmentation and Coulomb explosion of deuterium clusters by the interaction with intense laser pulses. Physical Review A, 2005, 72, .	2.5	15
121	Simulating the thermal behavior and fragmentation mechanisms of exohedral and substitutional silicon-doped C60. Journal of Chemical Physics, 2005, 123, 204323.	3.0	33
122	Theoretical study of the reactivity of cesium with benzene and graphitic CxHy clusters. Journal of Chemical Physics, 2005, 123, 074303.	3.0	7
123	Enhancement of hydrogen physisorption on graphene and carbon nanotubes by Li doping. Journal of Chemical Physics, 2005, 123, 204721.	3.0	247
124	Deformations and Thermal Stability of Carbon Nanotube Ropes. IEEE Nanotechnology Magazine, 2004, 3, 230-236.	2.0	27
125	Relativistic theory of an inhomogeneous electron liquid in relation to atomic binding energies. Physics and Chemistry of Liquids, 2004, 42, 589-595.	1.2	2
126	Excited states dynamics in time-dependent density functional theory. European Physical Journal D, 2004, 28, 211-218.	1.3	126

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127	Calculation of the optical spectrum of the Ti8C12 and V8C12 Met-Cars. Chemical Physics Letters, 2004, 398, 292-296.	2.6	12
128	Interaction of Molecular and Atomic Hydrogen With Single-Wall Carbon Nanotubes. IEEE Nanotechnology Magazine, 2004, 3, 304-310.	2.0	33
129	Interaction of lithium with graphene: Anab initiostudy. Physical Review B, 2004, 70, .	3.2	171
130	An Application of Non-Extensive Statistical Mechanics to Nanosystems. Journal of Computational and Theoretical Nanoscience, 2004, 1, 227-229.	0.4	42
131	Optical Properties of Nanostructures from Time-Dependent Density Functional Theory. Journal of Computational and Theoretical Nanoscience, 2004, 1, 231-255.	0.4	21
132	Growth Ability and Stability Indices of Clusters. Journal of Cluster Science, 2003, 14, 31-47.	3.3	7
133	Electronic metastable bound states of Mn22+ and Co22+. Chemical Physics Letters, 2003, 372, 82-89.	2.6	6
134	Metastable states in Au22+: a density functional study. Computational and Theoretical Chemistry, 2003, 639, 203-211.	1.5	3
135	Tight binding studies of exohedral silicon doped C60. Composites Science and Technology, 2003, 63, 1499-1505.	7.8	8
136	Structural and thermal properties of silicon-doped fullerenes. Journal of Chemical Physics, 2003, 119, 1127-1135.	3.0	39
137	Ab initiomolecular dynamics simulations of the two-step melting of NaSn. Physical Review B, 2003, 68, .	3.2	1
138	Analysis of the bonding and reactivity of H and the Al13 cluster using density functional concepts. Journal of Chemical Physics, 2003, 119, 5128-5141.	3.0	55
139	Coulomb explosion of deuterium cationic clusters. Physical Review A, 2003, 68, .	2.5	8
140	Interaction of molecular and atomic hydrogen with single-wall carbon nanotubes. , 2003, , .		1
141	Correlation energies of light atoms related to pairing between antiparallel spin electrons. Journal of Physics B: Atomic, Molecular and Optical Physics, 2003, 36, 2695-2705.	1.5	16
142	Deformations and thermal stability of carbon nanotube ropes. , 2003, , .		1
143	Patching and Tearing Single-Wall Carbon-Nanotube Ropes into Multiwall Carbon Nanotubes. Physical Review Letters, 2002, 89, 255501.	7.8	52
144	Can optical spectroscopy directly elucidate the ground state of C20?. Journal of Chemical Physics, 2002, 116, 1930-1933.	3.0	55

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145	Stability of aSn4tetrahedral cluster in an alkali atom environment. Physical Review B, 2002, 65, .	3.2	6
146	Behavior of the Surface Tension and the Viscosity in the Eutecticregion of the Liquid Feb alloy. Physics and Chemistry of Liquids, 2002, 40, 57-65.	1.2	2
147	Conditions for the self-assembling of cluster materials. Nanotechnology, 2002, 13, 253-257.	2.6	23
148	Some Properties of a Model Liquid of C 60 Buckyballs. Physics and Chemistry of Liquids, 2002, 40, 457-467.	1.2	3
149	Interaction of molecular and atomic hydrogen with (5,5) and (6,6) single-wall carbon nanotubes. Journal of Chemical Physics, 2002, 117, 2281-2288.	3.0	198
150	Octet composition in alkali-Pb solid alloys. Physical Review B, 2002, 66, .	3.2	1
151	Metastable phase stability in the ternary Zrâ€“Feâ€“Cr system. Intermetallics, 2002, 10, 205-216.	3.9	22
152	Amorphization in GdÂCo alloys and multilayers. Journal of Physics Condensed Matter, 2002, 14, 8913-8924.	1.8	16
153	Computer simulation of cluster assembling. International Journal of Quantum Chemistry, 2002, 86, 226-238.	2.0	18
154	Nonthermal fragmentation of C60. Chemical Physics Letters, 2002, 352, 154-162.	2.6	22
155	ELECTRONIC SHELL EFFECTS IN METAL CLUSTERS AND THEIR CONSEQUENCES FOR CLUSTER SELF-ASSEMBLING. , 2002, , 1476-1507.		2
156	Melting in Large Sodium Clusters:Â An Orbital-Free Molecular Dynamics Study. Journal of Physical Chemistry B, 2001, 105, 2386-2392.	2.6	55
157	Melting behavior of large disordered sodium clusters. European Physical Journal D, 2001, 15, 221-227.	1.3	29
158	Exchange energy density and some approximate exchange potentials obtained from Hartreeâ€“Fock theory of the ground state of the Be atom. Chemical Physics Letters, 2001, 343, 166-170.	2.6	6
159	Assembling of hydrogenated aluminum clusters. European Physical Journal D, 2001, 16, 285-288.	1.3	16
160	Novel Polygonized Single-Wall Carbon Nanotube Bundles. Physical Review Letters, 2001, 86, 3056-3059.	7.8	113
161	Magnetic interactions between small Ni clusters. Solid State Communications, 2000, 116, 309-314.	1.9	0
162	Theoretical evidence of bound metastable states in the doubly ionized nickel dimer Ni22+. Chemical Physics Letters, 2000, 332, 481-486.	2.6	8

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163	New perspectives of the weighted spin-density approximation: gradient corrections and the valence-only approach. Computational and Theoretical Chemistry, 2000, 501-502, 153-166.	1.5	1
164	Tight binding molecular dynamics studies of boron assisted nanotube growth. Journal of Chemical Physics, 2000, 113, 3814-3821.	3.0	37
165	Ab initiocalculation of the lattice distortions induced by substitutionalAgâ^'andCuâ^'impurities in alkali halide crystals. Physical Review B, 2000, 62, 3086-3092.	3.2	7
166	Computer simulation of the spreading of metallic clusters landing at grazing incidence on a metallic surface. Physical Review B, 2000, 62, 16031-16039.	3.2	10
167	Interaction of lithium atoms with graphitic walls. AIP Conference Proceedings, 2000, , .	0.4	0
168	Molecular dynamics study of cluster impact on the (001) and (110) surfaces of fcc metals. Computational Materials Science, 2000, 17, 515-519.	3.0	10
169	Density functional study of adsorption of molecular hydrogen on graphene layers. Journal of Chemical Physics, 2000, 112, 8114-8119.	3.0	261
170	Electronic and Atomic Structure, and Magnetism of Transition-Metal Clusters. Chemical Reviews, 2000, 100, 637-678.	47.7	495
171	Lowest excitation energy in atoms in the adiabatic approximation related to the single-particle kinetic energy functional. Journal of Physics B: Atomic, Molecular and Optical Physics, 1999, 32, 2173-2179.	1.5	9
172	Calculation of the Band Gap Energy and Study of Cross Luminescence in Alkaline-Earth Dihalide Crystals. Journal of the Physical Society of Japan, 1999, 68, 2829-2835.	1.6	21
173	Relation between transport and thermodynamic properties in liquidsp-electron metals near freezing. Physical Review E, 1999, 60, 4125-4129.	2.1	8
174	Molecular-dynamics study of the structural rearrangements of Cu and Au clusters softly deposited on a Cu(001) surface. Physical Review B, 1999, 60, 2908-2915.	3.2	59
175	Orbital-free molecular dynamics simulations of melting in Na8 and Na20: Melting in steps. Journal of Chemical Physics, 1999, 111, 6026-6035.	3.0	71
176	Ab initio study of B32 clusters: competition between spherical, quasiplanar and tubular isomers. Chemical Physics Letters, 1999, 311, 21-28.	2.6	105
177	Improved Charge Transfer at Carbon Nanotube Electrodes. Advanced Materials, 1999, 11, 154-157.	21.0	493
178	Simulating the thermal stability and phase changes of small carbon clusters and fullerenes. European Physical Journal D, 1999, 6, 221-233.	1.3	25
179	Assembling alkaliâ€"lead solid compounds from clusters. Journal of Chemical Physics, 1999, 111, 7053-7061.	3.0	10
180	Magnetic moments of. European Physical Journal D, 1999, 6, 235.	1.3	15

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181	Electronic Structure of Bimetallic Clusters Based on Alkali Elements. Springer Series in Cluster Physics, 1999, , 255-276.	0.3	0
182	Ab initio calculations for mixed clusters of lead and alkali elements, and implications for the structure of their solid and liquid alloys. Chemical Physics Letters, 1998, 289, 451-456.	2.6	17
183	Gradient correction to the exchange pair-correlation function of the weighted spin-density approximation in the density functional formalism. Chemical Physics Letters, 1998, 296, 307-312.	2.6	1
184	Comparative ab initio studies of small tin and lead clusters. Annalen Der Physik, 1998, 510, 107-119.	2.4	13
185	Mixed lead-alkali clusters in the gas phase and in liquid alloys. International Journal of Quantum Chemistry, 1998, 69, 341-348.	2.0	5
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