Julio A Alonso

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/6513327/publications.pdf

Version: 2024-02-01

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	Electronic and Atomic Structure, and Magnetism of Transition-Metal Clusters. Chemical Reviews, 2000, 100, 637-678.	47.7	495
2	Improved Charge Transfer at Carbon Nanotube Electrodes. Advanced Materials, 1999, 11, 154-157.	21.0	493
3	Nonlocal approximation to the exchange potential and kinetic energy of an inhomogeneous electron gas. Physical Review B, 1978, 17, 3735-3743.	3.2	288
4	Density functional study of adsorption of molecular hydrogen on graphene layers. Journal of Chemical Physics, 2000, 112, 8114-8119.	3.0	261
5	Enhancement of hydrogen physisorption on graphene and carbon nanotubes by Li doping. Journal of Chemical Physics, 2005, 123, 204721.	3.0	247
6	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
7	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
8	Ab InitioPhotoabsorption Spectra and Structures of Small Semiconductor and Metal Clusters. Physical Review Letters, 1996, 77, 247-250.	7.8	193
9	Interaction of lithium with graphene: Anab initiostudy. Physical Review B, 2004, 70, .	3.2	171
10	The optimum average nanopore size for hydrogen storage in carbon nanoporous materials. Carbon, 2007, 45, 2649-2658.	10.3	168
11	Determination of the glass-forming concentration range in binary alloys from a semiempirical theory: Application to Zr-based alloys. Physical Review B, 1987, 36, 3716-3722.	3.2	137
12	Molecular-dynamics study of the binding energy and melting of transition-metal clusters. Physical Review B, 1993, 48, 8253-8262.	3.2	132
13	Excited states dynamics in time-dependent density functional theory. European Physical Journal D, 2004, 28, 211-218.	1.3	126
14	Structural and dynamical properties of Cuâ€“Au bimetallic clusters. Journal of Chemical Physics, 1996, 104, 1056-1066.	3.0	122
15	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
16	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
17	Novel Polygonized Single-Wall Carbon Nanotube Bundles. Physical Review Letters, 2001, 86, 3056-3059.	7.8	113
18	Prediction of amorphous alloy formation by ion beam mixing. Solid State Communications, 1983, 48, 765-767.	1.9	106

#	Article	IF	Citations
19	Ab initio study of B32 clusters: competition between spherical, quasiplanar and tubular isomers. Chemical Physics Letters, 1999, 311, 21-28.	2.6	105
20	Adsorption and Dissociation of Molecular Hydrogen on Palladium Clusters Supported on Graphene. Journal of Physical Chemistry C, 2012, 116, 21179-21189.	3.1	104
21	Synthesis of fullerenes. Journal of Physical Organic Chemistry, 2013, 26, 526-539.	1.9	101
22	Molecular-dynamics study of the structures, binding energies, and melting of clusters of fcc transition and noble metals using the Voter and Chen version of the embedded-atom model. Physical Review B, 1994, 49, 8495-8498.	3.2	95
23	From graphene oxide to pristine graphene: revealing the inner workings of the full structural restoration. Nanoscale, 2015, 7, 2374-2390.	5.6	95
24	Construction of free-energy diagrams of amorphous alloys. Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics, 1990, 12, 587-595.	0.4	93
25	A non-local approximation to the exchange energy of the non-homogeneous electron gas. Solid State Communications, 1977, 24, 135-138.	1.9	88
26	Electronic and atomic structure of Na, Mg, Al and Pb clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1988, 11, 163-174.	1.0	85
27	Glass formation in ternary transition metal alloys. Journal of Physics Condensed Matter, 1990, 2, 6245-6250.	1.8	85
28	Density functional calculations of hydrogen adsorption on boron nanotubes and boron sheets. Nanotechnology, 2006, 17, 778-785.	2.6	83
29	Prediction of solid solubility in alloys. Physical Review B, 1980, 22, 5583-5589.	3.2	74
30	Magnetic moments of Ni clusters. Physical Review B, 1998, 57, 12469-12475.	3.2	73
31	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
32	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
33	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
34	Structure and bonding in small neutral alkali halide clusters. Physical Review B, 1997, 56, 15353-15360.	3.2	69
35	Simulation of the hydrogen storage in nanoporous carbons with different pore shapes. International Journal of Hydrogen Energy, 2011, 36, 10748-10759.	7.1	65
36	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

#	Article	IF	Citations
37	Stability and magic numbers of hetero-atomic clusters of simple metals. Physica B: Condensed Matter, 1988, 154, 73-81.	2.7	58
38	Interaction and concerted diffusion of lithium in a (5,5) carbon nanotube. Physical Review B, 2008, 78, .	3.2	58
39	Molecular-dynamics study of the structure, binding energy, and melting of small clusters of fullerene molecules using Girifalcoâ€™s spherical model. Physical Review B, 1994, 49, 8491-8494.	3.2	56
40	Melting in Large Sodium Clusters:Â An Orbital-Free Molecular Dynamics Study. Journal of Physical Chemistry B, 2001, 105, 2386-2392.	2.6	55
41	Can optical spectroscopy directly elucidate the ground state of C20?. Journal of Chemical Physics, 2002, 116, 1930-1933.	3.0	55
42	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
43	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
44	Density functional study of molecular hydrogen coverage on carbon nanotubes. Computational Materials Science, 2006, 35, 238-242.	3.0	54
45	Glass formation in binary alloy systems: A prediction of the composition range. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1988, 58, 79-92.	0.6	53
46	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
47	Patching and Tearing Single-Wall Carbon-Nanotube Ropes into Multiwall Carbon Nanotubes. Physical Review Letters, 2002, 89, 255501.	7.8	52
48	Electronegativity scale for metals. Physical Review B, 1979, 19, 3889-3895.	3.2	51
49	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
50	Embedded-atom method applied to bimetallic clusters: The Cu-Ni and Cu-Pd systems. Physical Review B, 1994, 49, 16649-16658.	3.2	50
51	Semiempirical Theory of Solid Solubility in Transition Metal Alloys. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1985, 40, 1199-1205.	1.5	49
52	Theoretical study of icosahedral Ni clusters within the embedded-atom method. Physical Review B, 1996, 54, 5961-5969.	3.2	49
53	Hydrogen storage capacities of nanoporous carbon calculated by density functional and MÃ¸ller-Plesset methods. Physical Review B, 2008, 78, .	3.2	49
54	Geometrical effects on the magnetism of small Ni clusters. Physical Review B, 1997, 55, 13279-13282.	3.2	48

#	Article	IF	Citations
55	Influence of nonlocal exchange-correlation effects on the response properties of simple metal clusters. Physical Review B, 1992, 46, 4891-4898.	3.2	47
56	Density-functional calculation of the fragmentation of doubly ionized spherical jelliumlike metallic microparticles. Physical Review B, 1986, 34, 2152-2157.	3.2	46
57	Prediction of the glass formation range of transition metal alloys. Journal of Physics F: Metal Physics, 1988, 18, 2149-2157.	1.6	46
58	Response properties of sodium clusters within a jellium-like model with finite surface thickness. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1991, 19, 93-96.	1.0	45
59	Competition between molecular and dissociative adsorption of hydrogen on palladium clusters deposited on defective graphene. RSC Advances, 2015, 5, 47945-47953.	3.6	45
60	Glass-forming ability in binary alloys produced by ion beam mixing and by laser quenching. Materials Letters, 1986, 4, 316-319.	2.6	44
61	A theoretical study of the static structure and thermodynamics of liquid lithium. Journal of Physics Condensed Matter, 1993, 5, 4283-4298.	1.8	44
62	Clusters and layers ofC60molecules supported on a graphite substrate. Physical Review B, 1997, 55, 7190-7197.	3.2	44
63	Weighted-density exchange and local-density Coulomb correlation energy functionals for finite systems: Application to atoms. Physical Review A, 1993, 48, 4197-4212.	2.5	42
64	Half-metallic finite zigzag single-walled carbon nanotubes from first principles. Physical Review B, 2008, 78, .	3.2	42
65	An Application of Non-Extensive Statistical Mechanics to Nanosystems. Journal of Computational and Theoretical Nanoscience, 2004, 1, 227-229.	0.4	42
66	Charge transfer and heat of formation in CsCl intermetallic compounds. Journal of Physics and Chemistry of Solids, 1978, 39, 79-87.	4.0	41
67	Nonlocality and the energy of alloy formation. Journal of Physics F: Metal Physics, 1978, 8, 2455-2460.	1.6	40
68	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
69	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
70	Adsorption and growth of palladium clusters on graphdiyne. Physical Chemistry Chemical Physics, 2017, 19, 19094-19102.	2.8	40
71	Coulomb barriers in the dissociation of doubly charged clusters. Physical Review B, 1991, 43, 9459-9466.	3.2	39
72	Structural and thermal properties of silicon-doped fullerenes. Journal of Chemical Physics, 2003, 119, 1127-1135.	3.0	39

#	Article	IF	Citations
73	Structural and thermal stability of narrow and short carbon nanotubes and nanostrips. Carbon, 2005, 43, 1371-1377.	10.3	38
74	Tight binding molecular dynamics studies of boron assisted nanotube growth. Journal of Chemical Physics, 2000, 113, 3814-3821.	3.0	37
75	Simulated porosity and electronic structure of nanoporous carbons. Journal of Chemical Physics, 2011, 135, 104706.	3.0	37
76	On the Factors Controlling Glass Forming Ability of Metallic Alloys Formed by Fast Liquid Quenching. Physica Status Solidi A, 1984, 81, 55-61.	1.7	35
77	Ab initiocalculations of structures and stabilities of(NaI)nNa+and(CsI)nCs+cluster ions. Physical Review B, 1998, 58, 9972-9979.	3.2	35
78	Comparative ab initio studies of small tin and lead clusters. Annalen Der Physik, 1998, 7, 107-119.	2.4	35
79	Theoretical study of the stability of AgN2+, AgN, AgN, AgNâ˜' and NaNâ˜' clusters as a function of size using the density functional formalism. Chemical Physics, 1988, 120, 239-247.	1.9	34
80	Theoretical study of the photoabsorption spectrum ofNa8,Na20,Cs8, andCs10O clusters. Physical Review B, 1992, 45, 13657-13663.	3.2	34
81	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
82	Adsorption of Lithium on Finite Graphitic Clusters. Journal of Physical Chemistry C, 2009, 113, 939-941.	3.1	34
83	The Atomic Size-Mismatch Contribution to the Enthalpy of Formation of Concentrated Substitutional Metallic Solid Solutions. Physica Status Solidi A, 1984, 85, 423-428.	1.7	33
84	Interaction of Molecular and Atomic Hydrogen With Single-Wall Carbon Nanotubes. IEEE Nanotechnology Magazine, 2004, 3, 304-310.	2.0	33
85	Simulating the thermal behavior and fragmentation mechanisms of exohedral and substitutional silicon-doped C60. Journal of Chemical Physics, 2005, 123, 204323.	3.0	33
86	The interaction of sulfuric acid with graphene and formation of adsorbed crystals. Nanotechnology, 2007, 18, 485705.	2.6	33
87	Magic numbers of sodium clusters. Solid State Communications, 1986, 57, 85-88.	1.9	31
88	Simulation of hydrogen storage in porous carbons. Journal of Materials Research, 2013, 28, 589-604.	2.6	31
89	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
90	Equivalence of ionization potential and magnitude of chemical potential in Hartreeâ€"Fock theory of atoms. Journal of Chemical Physics, 1983, 78, 1382-1383.	3.0	29

#	Article	IF	Citations
91	Surface plasmon excitations in C60, C60K and C60H clusters. Physica B: Condensed Matter, 1993, 183, 247-263.	2.7	29
92	Thermal road for fullerene annealing. Chemical Physics Letters, 1997, 273, 367-370.	2.6	29
93	Melting behavior of large disordered sodium clusters. European Physical Journal D, 2001, 15, 221-227.	1.3	29
94	Surface energy of liquid metals at the melting temperature related to bulk liquid structure. Surface Science, 1985, 160, 509-516.	1.9	28
95	Deformations and Thermal Stability of Carbon Nanotube Ropes. IEEE Nanotechnology Magazine, 2004, 3, 230-236.	2.0	27
96	Atomic structure and segregation in alkali-metal heteroclusters. Physical Review B, 1990, 42, 5000-5008.	3.2	26
97	A molecular dynamics study of the evaporation of small argon clusters. Physica B: Condensed Matter, 1992, 179, 273-277.	2.7	25
98	Theoretical Models for the Optical Properties of Clusters and Nanostructures. International Journal of Modern Physics B, 1997, 11, 2727-2776.	2.0	25
99	Theoretical Study of Small (NaI)nClusters. Journal of Physical Chemistry B, 1997, 101, 5944-5950.	2.6	25
100	Simulating the thermal stability and phase changes of small carbon clusters and fullerenes. European Physical Journal D, 1999, 6, 221-233.	1.3	25
101	Adsorption of hydrogen on normal and pentaheptite single wall carbon nanotubes. European Physical Journal D, 2005, 34, 279-282.	1.3	25
102	Theoretical study of molecular hydrogen clusters. European Physical Journal D, 2007, 43, 61-64.	1.3	25
103	Controlling the Adsorption of Carbon Monoxide on Platinum Clusters by Dopantâ€Induced Electronic Structure Modification. Angewandte Chemie, 2016, 128, 11225-11229.	2.0	25
104	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
105	Long-Range van der Waals Interactions in Density Functional Theory. Theoretical Chemistry Accounts, 2007, 117, 467-472.	1.4	24
106	Gradient corrections in the energy density functional. Chemical Physics Letters, 1978, 53, 190-191.	2.6	23
107	Prediction of solid solubility in alloys. Application to noble metal based alloys. Acta Metallurgica, 1982, 30, 105-107.	2.1	23
108	Conditions for the self-assembling of cluster materials. Nanotechnology, 2002, 13, 253-257.	2.6	23

#	Article	IF	Citations
109	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
110	Charge transfer in binary alloys and to impurities in iron. Journal of Physics and Chemistry of Solids, 1977, 38, 869-876.	4.0	22
111	Atomic electronegativity from density functional theory. Journal of Chemical Physics, 1980, 73, 1313-1319.	3.0	22
112	Dissociation channels ofNaN+clusters (3â‰Nâ‰37). Physical Review B, 1990, 41, 5595-5601.	3.2	22
113	Theoretical study of the binding of Na clusters encapsulated in theC240fullerene. Physical Review B, 1996, 53, 16059-16066.	3.2	22
114	Metastable phase stability in the ternary Zrâ€“Feâ€“Cr system. Intermetallics, 2002, 10, 205-216.	3.9	22
115	Nonthermal fragmentation of C60. Chemical Physics Letters, 2002, 352, 154-162.	2.6	22
116	Buckling in boron sheets and nanotubes. Physica Status Solidi (A) Applications and Materials Science, 2006, 203, 1105-1110.	1.8	22
117	First-Principles Structural and Electronic Characterization of Ordered SiO₂ Nanowires. Journal of Physical Chemistry C, 2012, 116, 18973-18982.	3.1	22
118	Electronic and cohesive properties of small sodium particles. Surface Science, 1983, 127, 367-376.	1.9	21
119	Structure and energetics ofNanâ^'xLix(nâ‰21) clusters. Physical Review B, 1990, 41, 5636-5642.	3.2	21
120	Evolution of the structural stability of large Cu, Ni, Pd, and Ag clusters with size: An analysis within the embedded atom method. Journal of Cluster Science, 1994, 5, 287-302.	3.3	21
121	Tight-binding study of the ionization of iron clusters. Physical Review B, 1996, 54, 3003-3006.	3.2	21
122	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
123	Competition between Palladium Clusters and Hydrogen to Saturate Graphene Vacancies. Journal of Physical Chemistry C, 2017, 121, 10843-10850.	3.1	21
124	Optical Properties of Nanostructures from Time-Dependent Density Functional Theory. Journal of Computational and Theoretical Nanoscience, 2004, 1, 231-255.	0.4	21
125	Theoretical study of (NaCl)n clusters. Physica B: Condensed Matter, 1995, 212, 329-342.	2.7	20
126	On the electronegativity parameters of the theory of heats of alloy formation. Solid State Communications, 1979, 31, 9-14.	1.9	19

#	Article	IF	Citations
127	Immersion of hydrogen atoms in aluminium clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1989, 13, 269-275.	1.0	19
128	Density functional study of neutral and charged sodium and lead clusters in the jellium model. Physica B: Condensed Matter, 1990, 167, 19-32.	2.7	19
129	Non-local exchange and local Coulomb correlation energy density functionals for finite many-electron systems. Chemical Physics Letters, 1993, 205, 348-353.	2.6	19
130	Nonlocal exchange and kinetic energy density functionals with correct asymptotic behavior for electronic systems. International Journal of Quantum Chemistry, 1994, 49, 171-184.	2.0	19
131	Theoretical study of the adsorption of hydrogen on cobalt clusters. Physical Chemistry Chemical Physics, 2018, 20, 21163-21176.	2.8	19
132	Polarizabilities of aluminium clusters. Solid State Communications, 1990, 75, 139-142.	1.9	18
133	Electronic structure of negatively charged aluminium clusters. Physica B: Condensed Matter, 1991, 168, 32-38.	2.7	18
134	Inhomogeneous contraction of interatomic distances in metallic clusters: Calculations forCsnandOCsn. Physical Review B, 1991, 44, 7273-7282.	3.2	18
135	Nonmetal-metal transition in Ni clusters. Solid State Communications, 1997, 104, 635-639.	1.9	18
136	Computer simulation of cluster assembling. International Journal of Quantum Chemistry, 2002, 86, 226-238.	2.0	18
137	New insights on the reaction mechanisms for CO oxidation on Au catalysts. Chemical Physics Letters, 2009, 468, 201-204.	2.6	18
138	Semi-empirical study of metastable alloys produced by ion implantation in metals. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1982, 45, 713-722.	0.6	17
139	Electronegativity of positive ions in the density functional theory. Zeitschrift FÃ¼r Physik A, 1982, 305, 31-37.	1.4	17
140	Dissociation of doubly charged alkali metal clusters. Annalen Der Physik, 1992, 504, 270-280.	2.4	17
141	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
142	Charging mechanism for the bond elongation observed in suspended chains of gold atoms. Physical Review B, 2005, 72, .	3.2	17
143	Ab initio studies of propene epoxidation on oxidized silver surfaces. Physical Chemistry Chemical Physics, 2014, 16, 26546-26552.	2.8	17
144	Absence of spillover of hydrogen adsorbed on small palladium clusters anchored to graphene vacancies. Applied Surface Science, 2021, 559, 149835.	6.1	17

#	Article	IF	Citations
145	Volume of formation and electronic configuration in dilute alloys. Journal of Physics and Chemistry of Solids, 1979, 40, 449-455.	4.0	16
146	Electron density in simple metals. Relation to bulk and surface properties. Journal of Physics F: Metal Physics, 1980, 10, 1995-2008.	1.6	16
147	Density functional-pseudopotential approach to the heat of formation in alloys of alkali metals. Journal of Physics F: Metal Physics, 1981, 11, 2045-2053.	1.6	16
148	Theory of the heat of formation in homovalent disordered solid alloys of non-transition metals. Journal of Physics F: Metal Physics, 1982, 12, 1907-1921.	1.6	16
149	Semiempirical theory of solid solubility in metallic alloys. Physica Status Solidi A, 1983, 76, 675-682.	1.7	16
150	Assembling of hydrogenated aluminum clusters. European Physical Journal D, 2001, 16, 285-288.	1.3	16
151	Amorphization in GdÂCo alloys and multilayers. Journal of Physics Condensed Matter, 2002, 14, 8913-8924.	1.8	16
152	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
153	Photoabsorption spectra of Ti8C12 metallocarbohedrynes: Theoretical spectroscopy within time-dependent density functional theory. Journal of Chemical Physics, 2006, 125, 074311.	3.0	16
154	Lifetime of electronic excitations in metal nanoparticles. New Journal of Physics, 2010, 12, 053023.	2.9	16
155	One-Electron Energy Eigenvalues in the Weighted-Density Approximation to Exchange and Correlation. Europhysics Letters, 1991, 14, 323-329.	2.0	15
156	Fragmentation and Coulomb explosion of deuterium clusters by the interaction with intense laser pulses. Physical Review A, 2005, 72, .	2.5	15
157	Electronic and atomic structure of the AlnHn+2 clusters. Journal of Chemical Physics, 2008, 129, 074306.	3.0	15
158	Surfactant effect of sulfuric acid on the exfoliation of bilayer graphene. Physical Review B, 2011, 84, .	3.2	15
159	Adsorption and dissociation of molecular hydrogen on the edges of graphene nanoribbons. Journal of Nanoparticle Research, 2012, 14, 1.	1.9	15
160	Cathodoluminescence in single and multiwall WS2 nanotubes: Evidence for quantum confinement and strain effect. Applied Physics Reviews, 2020, 7, .	11.3	15
161	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
162	Magnetic moments of. European Physical Journal D, 1999, 6, 235.	1.3	15

#	Article	IF	Citations
163	Charge transfer in simple metallic alloys. Journal De Physique, 1983, 44, 229-234.	1.8	14
164	X-ray scattering factors of crystalline silicon and germanium from A bond charge model. Journal of Physics and Chemistry of Solids, 1988, 49, 1013-1017.	4.0	14
165	Electronic structure of CsN and CsNO clusters. Solid State Communications, 1989, 71, 591-594.	1.9	14
166	Theoretical study of NaCl clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1993, 26, 213-215.	1.0	14
167	Nonlocal exchange- and kinetic-energy density functionals for electronic systems: Application to atoms and ions. Physical Review A, 1993, 47, 1804-1810.	2.5	14
168	Self-consistent local-density approximation with model Coulomb pair-correlation functions for electronic systems. Physical Review A, 1993, 47, 1811-1816.	2.5	14
169	Deformed-jellium model for the fission of multiply charged simple metal clusters. Physical Review B, 1995, 51, 1897-1901.	3.2	14
170	Interaction of the Charged Deuterium Cluster D3+with Femtosecond Laser Pulsesâ€. Journal of Physical Chemistry C, 2007, 111, 17765-17772.	3.1	14
171	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
172	Ab initio studies of ethanol dehydrogenation at binary AuPd nanocatalysts. Molecular Catalysis, 2018, 449, 8-13.	2.0	14
173	Partial Pressure Contributions to the Equation of State of Alkali Metals. Physica Status Solidi (B): Basic Research, 1980, 100, 701-704.	1.5	13
174	Semiempirical calculation of the surface dipole barrier in metals. Solid State Communications, 1980, 33, 59-62.	1.9	13
175	Electronegativity equalization and electron transfer in molecules. Molecular Physics, 1983, 48, 981-988.	1.7	13
176	Nonlocal density functional calculation of the electron affinity of atoms. Physics Letters, Section A: General, Atomic and Solid State Physics, 1986, 114, 236-240.	2.1	13
177	Coulomb explosion of charged jellium clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1989, 11, 323-326.	1.0	13
178	Distribution of interatomic distances in large metallic clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1992, 22, 541-545.	1.0	13
179	Collective electronic excitations in metal-coatedC60. Physical Review B, 1994, 49, 17397-17402.	3.2	13
180	An experimental and theoretical study of the glass-forming region of the Mg-Cu-Sn system. Journal of Materials Science, 1995, 30, 40-46.	3.7	13

#	Article	IF	Citations
181	Comparative ab initio studies of small tin and lead clusters. Annalen Der Physik, 1998, 510, 107-119.	2.4	13
182	Lattice distortions around aTl+impurity inNaI:Tl+andCsI:Tl+scintillators: Anab initiostudy involving large active clusters. Physical Review B, 1998, 58, 11964-11969.	3.2	13
183	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
184	Stability of silicon-doped C60 dimers. Journal of Chemical Physics, 2007, 126, 044705.	3.0	13
185	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
186	Observation of Zr22+, Cd22+, Hf22+, W22+, and Pt22+ in the gas phase. Journal of Chemical Physics, 2009, 130, 144312.	3.0	13
187	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
188	A theory of order-Disorder and antiphase domain boundary energies. Metallurgical and Materials Transactions A - Physical Metallurgy and Materials Science, 1980, 11, 1747-1753.	1.4	12
189	Volume Dependence of the Bulk Modulus in Alkali Metals. Physica Status Solidi (B): Basic Research, 1981, 104, 307-312.	1.5	12
190	Local behavior of the kinetic energy in density functional theory. International Journal of Quantum Chemistry, 1985, 27, 393-406.	2.0	12
191	Dissociation energy of alkali metal clusters related to inhomogeneous electron gas theory. Molecular Physics, 1993, 79, 393-403.	1.7	12
192	Atomic structure of metallic clusters of large size. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1994, 69, 1045-1050.	0.6	12
193	Calculation of the optical spectrum of the Ti8C12 and V8C12 Met-Cars. Chemical Physics Letters, 2004, 398, 292-296.	2.6	12
194	Theoretical study of the photoabsorption spectrum of small chromium clusters. Physical Review B, 2007, 76, .	3.2	12
195	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
196	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
197	Dynamics of Cluster Isomerization Induced by Hydrogen Adsorption. Journal of Physical Chemistry C, 2019, 123, 15236-15243.	3.1	12
198	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

#	Article	IF	Citations
199	Semi-statistical model for metals. Journal of Physics and Chemistry of Solids, 1977, 38, 307-310.	4.0	11
200	Density Functional theory of the atomic electronegativity. Zeitschrift FÃ¼r Physik A, 1981, 302, 307-310.	1.4	11
201	A non local approximation to the correlation energy of inhomogeneous electron systems. Physics Letters, Section A: General, Atomic and Solid State Physics, 1981, 81, 467-469.	2.1	11
202	Study of an approximate relation between the energy of an atom and the electronic potential at the nucleus. International Journal of Quantum Chemistry, 1982, 22, 989-997.	2.0	11
203	Electronic and elastic effects in the interaction of impurities in ternary metallic alloys. Journal of Physics and Chemistry of Solids, 1985, 46, 1147-1151.	4.0	11
204	On the Concentration Dependence of the Ordering Potential in Liquid Li-Pb Alloys. Physics and Chemistry of Liquids, 1987, 16, 249-258.	1.2	11
205	Stability and magic numbers of small KxMg clusters. Journal of Physics F: Metal Physics, 1987, 17, L197-L200.	1.6	11
206	Nonlocal exchange and kinetic-energy density functionals for electronic systems. International Journal of Quantum Chemistry, 1992, 44, 347-358.	2.0	11
207	Stabilities of large sodium clusters for different atomic arrangements. Physical Review B, 1993, 47, 4747-4755.	3.2	11
208	Thermodynamic analysis of irradiation-induced amorphization of intermetallic particles in Zircaloy. Journal of Materials Science, 1995, 30, 196-200.	3.7	11
209	Exchange and correlation in density functional theory. International Journal of Quantum Chemistry, 1995, 56, 49-59.	2.0	11
210	Free-energies of the Ti-Ni, Fe-Ni and Mo-Ni alloys in relation to their behaviour under particle irradiation. Journal of Materials Science, 1996, 31, 6395-6402.	3.7	11
211	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
212	Concentration fluctuations in simple metallic liquid alloys. Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics, 1982, 114, 67-70.	0.9	10
213	Cohesive energy of small metallic particles. Solid State Communications, 1984, 50, 549-552.	1.9	10
214	Theory of the thermodynamic properties of binary mixtures of organic molecules with size mismatch. Chemical Physics, 1985, 99, 35-41.	1.9	10
215	Surface Energy of Liquid Transition Metals Related to Bulk Compressibility and Thickness. Physics and Chemistry of Liquids, 1987, 17, 209-214.	1.2	10
216	Possibility of spontaneous vitrification in Ti-Cr alloys. Physica B: Condensed Matter, 1989, 160, 108-112.	2.7	10

#	Article	IF	Citations
217	Glass formation in the Cuâ€“Tiâ€“Zr system and its associated binary systems. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1992, 65, 989-1000.	0.6	10
218	Theoretical calculation of the amorphous alloy range of the Mg-Cu system. Journal of Materials Science, 1992, 27, 4935-4939.	3.7	10
219	Nonlocal approximation to the exchange and kinetic energy functionals: Application to metallic clusters. International Journal of Quantum Chemistry, 1993, 45, 333-347.	2.0	10
220	Atomic structure and collective excitations of medium size NanKm clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1993, 28, 311-319.	1.0	10
221	Variation of the ground-state correlation energy of atoms with atomic number. Journal of Physics B: Atomic, Molecular and Optical Physics, 1996, 29, 1629-1636.	1.5	10
222	Assembling alkaliâ€“lead solid compounds from clusters. Journal of Chemical Physics, 1999, 111, 7053-7061.	3.0	10
223	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
224	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
225	Structural corrections to Stokes-Einstein relation for liquid metals near freezing. Physical Review E, 2006, 73, 032201.	2.1	10
226	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
227	Interaction of aromatic molecules with small gold clusters. Chemical Physics Letters, 2017, 684, 91-96.	2.6	10
228	Ionization potentials of atoms calculated with a nonlocal exchange and a local correlation functional. International Journal of Quantum Chemistry, 1994, 52, 993-1010.	2.0	9
229	Density functional calculation of the photoabsorption spectrum of simple metal clusters: Beyond the local-density approximation and jellium model. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1994, 69, 1037-1044.	0.6	9
230	Theoretical study of gasâ€phase NanPb clusters and implications for liquid Naâ€“Pb alloys. Journal of Chemical Physics, 1996, 104, 8043-8047.	3.0	9
231	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
232	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
233	Palladium clusters, free and supported on surfaces, and their applications in hydrogen storage. Physical Chemistry Chemical Physics, 2022, 24, 2729-2751.	2.8	9
234	Density functional calculation of the ionization potentials of small metallic particles. European Physical Journal B, 1985, 59, 187-191.	1.5	8

#	Article	IF	Citations
235	A non local density functional calculation of the diamagnetic susceptibilities and other electronic properties of noble gases and closed-shell ions. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1987, 6, 219-226.	1.0	8
236	Electronic and atomic structure of Cs N and Cs N O clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1990, 17, 203-208.	1.0	8
237	Barrier for the reactionX20++X20+â†'X402+in alkali-metal clusters related to electron density at the bond midpoint of the supermolecule (X20+)2. Physical Review B, 1994, 49, 5565-5569.	3.2	8
238	Incipient manifestation of the shell structure of atoms within the WDA model for the exchange and kinetic energy density functionals. Chemical Physics, 1995, 196, 455-463.	1.9	8
239	Building alkali-lead intermetallic compounds from clusters. Solid State Communications, 1998, 108, 519-524.	1.9	8
240	Relation between transport and thermodynamic properties in liquidsp-electron metals near freezing. Physical Review E, 1999, 60, 4125-4129.	2.1	8
241	Theoretical evidence of bound metastable states in the doubly ionized nickel dimer Ni22+. Chemical Physics Letters, 2000, 332, 481-486.	2.6	8
242	Tight binding studies of exohedral silicon doped C60. Composites Science and Technology, 2003, 63, 1499-1505.	7.8	8
243	Coulomb explosion of deuterium cationic clusters. Physical Review A, 2003, 68, .	2.5	8
244	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
245	Electronic and magnetic properties of Fe clusters inside finite zigzag single-wall carbon nanotubes. Physical Review B, 2013, 87, .	3.2	8
246	An improved descriptor of cluster stability: application to small carbon clusters. Physical Chemistry Chemical Physics, 2018, 20, 27368-27374.	2.8	8
247	Bimetallic Alâ€“Sn clusters: mixing at the nanoscale. Physical Chemistry Chemical Physics, 2019, 21, 22919-22929.	2.8	8
248	Reactivity of Cobaltâ€Fullerene Complexes towards Deuterium. ChemPhysChem, 2020, 21, 1012-1018.	2.1	8
249	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
250	Semiempirical Study of Metastable Alloys Obtained by Ion Implantation in Metals and Semiconductors. Physica Status Solidi A, 1982, 72, 777-781.	1.7	7
251	Simple charge transfer model of X-ray scattering by ten-electron molecules. Molecular Physics, 1983, 50, 789-796.	1.7	7
252	Simple density functional theory of the electronegativity and other related properties of atoms and ions. , 1987, , 41-78.		7

#	Article	IF	Citations
253	Size effects on the vacancy-formation energy of small sodium clusters in the jellium model. Physical Review B, 1988, 37, 8436-8439.	3.2	7
254	Enrichment and segregation in alkali heteroclusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1989, 12, 237-239.	1.0	7
255	Surface Thickness of Liquid Metals Related to Surface Energy and Bulk Compressibility: A Universal Relation. Physics and Chemistry of Liquids, 1990, 21, 257-259.	1.2	7
256	Stability of isomeric Na n clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1991, 19, 141-143.	1.0	7
257	Fission barriers for Na N 2+ cluster dissociation. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1994, 31, 275-277.	1.0	7
258	Vibrational frequencies of sodium clusters. International Journal of Quantum Chemistry, 1995, 56, 589-601.	2.0	7
259	Charge transfer within zintl ions in liquid metallic alloys. A cluster study. Computational and Theoretical Chemistry, 1995, 330, 267-272.	1.5	7
260	Theoretical study of the collective electronic excitations in single- and multiple-shell fullerenes. Physical Review B, 1995, 52, 8446-8453.	3.2	7
261	Density functional theory of clusters of nontransition metals using simple models. Topics in Current Chemistry, 1996, , 119-171.	4.0	7
262	Structure, transport and surface properties of dense fluids, especially liquid metals. Molecular Physics, 1998, 95, 353-361.	1.7	7
263	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
264	Growth Ability and Stability Indices of Clusters. Journal of Cluster Science, 2003, 14, 31-47.	3.3	7
265	Theoretical study of the reactivity of cesium with benzene and graphitic CxHy clusters. Journal of Chemical Physics, 2005, 123, 074303.	3.0	7
266	Ionization potentials of neutral atoms and positive ions in the limit of large atomic number. Physical Review A, 2007, 75, .	2.5	7
267	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
268	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
269	Interaction of hydrogen with palladiumâ€“copper nanoalloys. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	7
270	C60Con complexes as hydrogen adsorbing materials. International Journal of Hydrogen Energy, 2021, 46, 20594-20606.	7.1	7

#	Article	IF	Citations
271	Infrared spectra and structures of C60Rhn+ complexes. Carbon, 2022, 197, 535-543.	10.3	7
272	Relation of Regular Solution Theory of Liquid Metal Alloys to Miedema's Work. Physics and Chemistry of Liquids, 1981, 11, 135-139.	1.2	6
273	Electronegativity of fractionally charged atoms in the Density Functional Theory. Zeitschrift FÃ¼r Physik A, 1983, 312, 95-98.	1.4	6
274	Density functional estimates of charge transfer and chemical potentials in hydrogen halides and mixed halides. Chemical Physics, 1983, 76, 121-124.	1.9	6
275	Concentration dependence of the heat of formation of binary liquid alloys. Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics, 1983, 122, 23-27.	0.9	6
276	Density functional calculation of the electronegativity and other related properties of atoms and ions of the principal groups of the periodic table. Zeitschrift FÃ¼r Physik A, 1984, 319, 275-282.	1.4	6
277	Density functional theory of the chemical potential of atoms and its relation to electrostatic potentials and bonding distances. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1986, 1, 215-221.	1.0	6
278	Determination of phase diagrams of eutectic binary alloys with partial solid solubility. Physica B: Condensed Matter, 1988, 154, 82-86.	2.7	6
279	Electronic structure and stability of KxMg clusters. Comparison between the jellium-on-jellium model and an improved model. Physics Letters, Section A: General, Atomic and Solid State Physics, 1989, 140, 67-71.	2.1	6
280	Atomic and electronic structure of Na10K10Cs n clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1994, 30, 349-356.	1.0	6
281	Density functional theory of the structure of bimetallic clusters. Physica Scripta, 1994, T55, 177-182.	2.5	6
282	Density functional theory of the collective electronic excitations in NanKnclusters. International Journal of Quantum Chemistry, 1995, 56, 839-846.	2.0	6
283	Thermal behaviour of carbon clusters and small fullerenes. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1997, 40, 385-388.	1.0	6
284	Study of clusters of interest for liquid ionic alloys. Annalen Der Physik, 1997, 509, 35-44.	2.4	6
285	Ionic vibrational breathing mode of metallic clusters. International Journal of Quantum Chemistry, 1997, 61, 613-626.	2.0	6
286	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
287	Stability of aSn4tetrahedral cluster in an alkali atom environment. Physical Review B, 2002, 65, .	3.2	6
288	Electronic metastable bound states of Mn22+ and Co22+. Chemical Physics Letters, 2003, 372, 82-89.	2.6	6

#	Article	IF	Citations
289	A density-functional study on the formation of Mo22+. Journal of Chemical Physics, 2005, 123, 134313.	3.0	6
290	BeB2nanostructures: A density functional study. Physical Review B, 2005, 72, .	3.2	6
291	Interaction of narrow carbon nanotubes with nitronium tetrafluoroborate salts. Journal of Chemical Physics, 2008, 128, 214703.	3.0	6
292	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
293	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
294	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
295	Structure, stability and optical absorption spectra of small TinCx clusters: a first-principles approach. Monthly Notices of the Royal Astronomical Society, 0, , .	4.4	6
296	Surface dipole barrier in metals. Relation to the bulk electron density. Zeitschrift FÃ¼r Physik B Condensed Matter and Quanta, 1981, 40, 307-309.	1.9	5
297	Density functional pseudopotential calculation of the cohesive properties of disordered solid alloys of nontransition metals application to Znâ€”Cd. Physica Status Solidi (B): Basic Research, 1983, 119, 589-594.	1.5	5
298	On the chemical potential of atomic ions. Physics Letters, Section A: General, Atomic and Solid State Physics, 1984, 101, 20-22.	2.1	5
299	A note on the entropy of mixing of liquid sodium-caesium and other binary alkali alloys. Journal of Physics F: Metal Physics, 1985, 15, L185-L188.	1.6	5
300	Asymmetric rare gas pair potentials from energy density functionals. Journal of Chemical Physics, 1986, 85, 6637-6644.	3.0	5
301	Correlation of Glass Forming Ability with Thermochemical Coordinates*. Zeitschrift Fur Physikalische Chemie, 1988, 156, 109-113.	2.8	5
302	Electronic and atomic structure of simple-metal clusters: Beyond the spherical jellium model. , 1992, , 327-334.		5
303	Photoabsorption cross sections of sodium clusters: electronic and geometrical effects. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1993, 26, 284-286.	1.0	5
304	Potential energy curve of H+2related to mirror-plane ground-state electron density. Molecular Physics, 1993, 79, 1143-1146.	1.7	5
305	Semi-empirical model for the fission of multiply charged metal clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1995, 33, 301-305.	1.0	5
306	Mixed lead-alkali clusters in the gas phase and in liquid alloys. International Journal of Quantum Chemistry, 1998, 69, 341-348.	2.0	5

#	Article	IF	Citations
307	Electrostrictive deformations in small carbon clusters, hydrocarbon molecules, and carbon nanotubes. Physical Review A, 2006, 74, .	2.5	5
308	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
309	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
310	The diatomic dication CuZn2+ in the gas phase. Journal of Chemical Physics, 2011, 135, 034306.	3.0	5
311	On the derivation of the SchrÃ¶dinger equation from Newtonian mechanics. Physics Letters, Section A: General, Atomic and Solid State Physics, 1972, 38, 501-502.	2.1	4
312	Solubility in nontransition homovalent alloys. Relation to the ionic radius. Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics, 1981, 103, 333-339.	0.9	4
313	Density functional-pseudopotential calculation of the heat of formation of disordered solid alkaline-earth alloys. Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics, 1982, 112, 73-77.	0.9	4
314	Density functional theory of asymptotic form of electron density in heteronuclear diatomic molecules. Journal of Chemical Physics, 1983, 79, 1903-1905.	3.0	4
315	Liquidus Curves of Eutectic NaK and NaCs Systems. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1984, 39, 842-845.	1.5	4
316	Role of the Excess Volume of Formation on Alloying. Physica Status Solidi (B): Basic Research, 1984, 123, 485-489.	1.5	4
317	Density Functional Pseudopotential Calculation of the Cohesive Properties of Disordered Solid Alloys of Alkalineâ€Earth Metals. Influence of the Ionic Pseudopotential. Physica Status Solidi (B): Basic Research, 1985, 129, 483-488.	1.5	4
318	A hard-sphere description of the thermodynamic properties of binary mixtures of organic molecules. Chemical Physics, 1986, 103, 35-42.	1.9	4
319	Charge transfer within clusters in liquid ionic alloys. Journal of Physics Condensed Matter, 1993, 5, 4271-4282.	1.8	4
320	Molecular dynamics study of A18B lennard-jones clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1994, 31, 299-301.	1.0	4
321	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
322	Adsorption of transition metal clusters on Boron-graphdiyne. Applied Surface Science, 2021, 548, 149270.	6.1	4
323	The virial, boundary kinetic-energy density and electron density, in one dimension and in spherical symmetry. Physics Letters, Section A: General, Atomic and Solid State Physics, 1981, 83, 455-456.	2.1	3
324	Cellular density functional theory of the heat of formation of disordered simple alloys. Physica Status Solidi (B): Basic Research, 1982, 114, 495-501.	1.5	3

#	Article	IF	Citations
325	Relation between total energy, electronic potential at the nucleus, and chemical potential of positive ions. International Journal of Quantum Chemistry, 1984, 26, 145-149.	2.0	3
326	Electron density and atomic relaxation around a vacancy in a small metal particle. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1986, 2, 177-181.	1.0	3
327	Vacancy Formation Energy in Close-packed Metals Connected with Liquid Thermodynamics at Melting. Physics and Chemistry of Liquids, 1989, 20, 235-240.	1.2	3
328	Evaporation rates of hot sodium clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1991, 20, 119-122.	1.0	3
329	Hardness of metallic clusters. , 1993, , 229-257.		3
330	Behaviour of the ionization potential at the closing of atomic shells in large b.c.c.-like spherical sodium clusters. Solid State Communications, 1995, 94, 799-803.	1.9	3
331	Electrostatic potential at the nucleus of a neutral atom related to electronic correlation energies of atomic ions. Molecular Physics, 1996, 88, 1365-1371.	1.7	3
332	ON THE FISSION OF CHARGED ALKALI-METAL CLUSTERS. Surface Review and Letters, 1996, 03, 617-621.	1.1	3
333	Density functional study of atomic electron affinities using a nonlocal exchange and a local correlation functional. International Journal of Quantum Chemistry, 1997, 61, 253-261.	2.0	3
334	Some Properties of a Model Liquid of C 60 Buckyballs. Physics and Chemistry of Liquids, 2002, 40, 457-467.	1.2	3
335	Metastable states in Au22+: a density functional study. Computational and Theoretical Chemistry, 2003, 639, 203-211.	1.5	3
336	Evolution of the atomic structure and the magnetism of small oxygen clusters. Computational and Theoretical Chemistry, 2013, 1021, 215-221.	2.5	3
337	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
338	Hydrogen quenches the size effects in carbon clusters. Physical Chemistry Chemical Physics, 2019, 21, 10402-10410.	2.8	3
339	Dimerization of pentacyclopentacorannulene C30H10 as a strategy to produce C60H20 as a precursor for C60. RSC Advances, 2020, 10, 3689-3693.	3.6	3
340	Ab initio study of (NaCl)nNA+ clusters. Canadian Journal of Physics, 1998, 76, 311-320.	1.1	3
341	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
342	A comparison of two parametrizations of solid solubility in alloys: Thermochemical coordinates versus orbital radii coordinates. Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics, 1982, 113, 103-112.	0.9	2

#	Article	IF	Citations
343	Relation between total energy, electronic potential at the nucleus and chemical potential. Application to the helium isoelectronic series in Hartree-Fock theory. Physics Letters, Section A: General, Atomic and Solid State Physics, 1983, 95, 89-91.	2.1	2
344	Concentration Fluctuations in Liquid Sodium-Caesium Alloys. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1984, 39, 596-599.	1.5	2
345	Liquidus Curves of Eutectic Naï£¿K and Naï£¿Cs Systems from Semiempirical Theories of Mixtures. Physica Status Solidi A, 1985, 89, 73-78.	1.7	2
346	Concentration Fluctuations in Binary Mixtures of Inert-Gas Fluids. Physics and Chemistry of Liquids, 1985, 15, 41-48.	1.2	2
347	Fragmentation channels of neutral and charged sodium clusters. Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics, 1988, 147, 243-248.	0.9	2
348	Nonlocal functionals for exchange and correlation in density functional theory: Application to atoms and to small atomic clusters. International Journal of Quantum Chemistry, 1995, 56, 499-508.	2.0	2
349	Screening of an Ion in a Finite Electron Gas and its Relation to Cluster Structure. Physics and Chemistry of Liquids, 1995, 29, 23-30.	1.2	2
350	Density functional pseudopotential study of the endohedral complex Li2@C60. Physica B: Condensed Matter, 1997, 240, 154-166.	2.7	2
351	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
352	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
353	High-pressure behaviour of crystalline silane compared with that for SnH4. Phase Transitions, 2009, 82, 247-250.	1.3	2
354	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
355	Elimination vs Substitution Reaction. A Dichotomy between BrÃ¸nstedâ€“Lowry and Lewis Basicity. Organic Letters, 2015, 17, 767-769.	4.6	2
356	Electronic and Atomic Structure of NanZn Clusters in the Spherically Averaged Pseudopotential Model. , 1991, , 373-386.		2
357	Fragmentation of Doubly Charged Alkali-Metal Clusters. Springer Series in Nuclear and Particle Physics, 1992, , 305-311.	0.1	2
358	Prediction of Metastable Alloy Formation and Phase Transformations Induced by Ion Bombardment in Binary Metal Systems. , 1992, , 328-335.		2
359	PREDICTION OF GLASS FORMATION BY SOLID STATE REACTION IN ALLOYS. Journal De Physique Colloque, 1990, 51, C4-111-C4-117.	0.2	2
360	ELECTRONIC SHELL EFFECTS IN METAL CLUSTERS AND THEIR CONSEQUENCES FOR CLUSTER SELF-ASSEMBLING. , 2002, , 1476-1507.		2

#	Article	IF	Citations
361	The Storage of Hydrogen in Nanoporous Carbons. Journal of the Mexican Chemical Society, 2017, 56, .	0.6	2
362	Concentration asymmetry and carbon enrichment in titanium carbide and silicon carbide clusters. Physical Review A, 2022, 105, .	2.5	2
363	Partial pressure contributions to the equation of state of alkaline-earth metals. Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics, 1982, 112, 67-72.	0.9	1
364	On the free energy of mixing of a binary liquid alloy. Physics and Chemistry of Liquids, 1983, 12, 265-268.	1.2	1
365	Construction of liquidus curves of simple-eutectic binary alloys from Miedema theory. Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics, 1988, 150, 369-377.	0.9	1
366	Atomic structure of metallic clusters of medium size. International Journal of Modern Physics B, 1992, 06, 3613-3621.	2.0	1
367	Phenomenology of Metallic Resistivity Observed in Single-Wall Nanotube Ropes as a Strongly Coupled ?-Electron C Ion Plasma. Physica Status Solidi (B): Basic Research, 1997, 203, 179-182.	1.5	1
368	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
369	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
370	Octet composition in alkali-Pb solid alloys. Physical Review B, 2002, 66, .	3.2	1
371	Ab initiomolecular dynamics simulations of the two-step melting of NaSn. Physical Review B, 2003, 68, .	3.2	1
372	Interaction of molecular and atomic hydrogen with single-wall carbon nanotubes. , 2003, , .		1
373	Deformations and thermal stability of carbon nanotube ropes. , 2003, , .		1
374	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
375	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
376	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
377	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
378	Metallicity enhancement in coreâ€“shell SiO2@RuO2nanowires. RSC Advances, 2014, 4, 34696-34700.	3.6	1

#	Article	IF	Citations
379	The diatomic dication SiC2+ in the gas phase. Chemical Physics, 2015, 455, 41-47.	1.9	1
380	Theoretical Study of the Metal-Nonmetal Transition in Transition Metal Clusters. , 1998, , 109-117.		1
381	A Combination of the Work Formalism for Exchange with an Optimized Correlation Energy Functional for Atoms. Journal De Physique II, 1995, 5, 1277-1287.	0.9	1
382	Density approximation to the average Hartree-Fock exchange potential for atoms. Journal of Chemical Sciences, 1994, 106, 91-102.	1.5	1
383	Simple model for liquid metal alloys and relation to Miedema's variables. Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics, 1982, 114, 141-146.	0.9	0
384	Clusters of Fullerene Molecules. Materials Science Forum, 1996, 232, 155-172.	0.3	0
385	Magnetic interactions between small Ni clusters. Solid State Communications, 2000, 116, 309-314.	1.9	0
386	Interaction of lithium atoms with graphitic walls. AIP Conference Proceedings, 2000, , .	0.4	0
387	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
388	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
389	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
390	Model for the Formation of Helium Bubbles in Palladium. Croatica Chemica Acta, 2013, 86, 425-429.	0.4	0
391	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
392	Interaction of hydrogen with palladium clusters deposited on graphene. AIP Conference Proceedings, 2015, , .	0.4	0
393	Interaction of Hydrogen with Graphitic Surfaces, Clean and Doped with Metal Clusters. , 2018, , 1-22.		0
394	Theoretical Study of the Diels-Alder Dimerization of C30H10. ECS Meeting Abstracts, 2021, MA2021-01, 645-645.	0.0	0
395	Density Functional Calculation of the Fragmentation of Neutral, Singly and Doubly-Ionized Spherical Jellium-Like Metallic Microparticles. , 1987, , 263-267.		0
396	Enrichment and segregation in alkali heteroclusters. , 1989, , 237-239.		0

#	Article	IF	Citations
397	Evaporation rates of hot sodium clusters. , 1991, , 569-572.		0
398	Fission barriers for Na N 2+ cluster dissociation. , 1995, , 231-234.		0
399	Theoretical Study of the Collective Electronic Excitations of the Endohedral Clusters Na N @C780. , 1998, , 133-141.		0
400	Electronic Structure of Bimetallic Clusters Based on Alkali Elements. Springer Series in Cluster Physics, 1999, , 255-276.	0.3	0
401	Hydrogen Interaction with Tungsten Disulfide Nanostructures. , 2021, , .		0
402	Interaction of Hydrogen with Graphitic Surfaces, Clean and Doped with Metal Clusters. , 2020, , 545-566.		0
403	Dissociation of doubly-charged alkali-metal clusters. , 1992, , 112-117.		0
404	Concentration Fluctuations in Liquid Alloys of Alkali Metals from Semiempirical Theories of Mixtures. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1985, 40, 425-429.	1.5	0
405	Symmetric and asymmetric fission of charged sodium clusters. Acta Physica Hungarica A Heavy Ion Physics, 1995, 1, 227-240.	0.4	0
406	Electrostatic potential at the nucleus of a neutral atom related to electronic correlation energies of atomic ions. Molecular Physics, 1996, 88, 1365-1372.	1.7	0