Julio A Alonso

List of Publications by Year in Descending Order

394 papers	9,508 citations	47 h-index	81 g-index
413 ext. papers	10,044 ext. citations	3.3 avg, IF	6.08 L-index

#	Paper	IF	Citations
394	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	2.5	6
393	Interaction of hydrogen with palladium□copper nanoalloys. *Theoretical Chemistry Accounts*, **2021**, 140, 1	1.9	3
392	Adsorption of transition metal clusters on Boron-graphdiyne. *Applied Surface Science*, **2021**, 548, 149270	6.7	0
391	C60Con complexes as hydrogen adsorbing materials. *International Journal of Hydrogen Energy*, **2021**, 46, 20594-20606	6.7	1
390	Absence of spillover of hydrogen adsorbed on small palladium clusters anchored to graphene vacancies. *Applied Surface Science*, **2021**, 559, 149835	6.7	1
389	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	4.6	7
388	Dimerization of pentacyclopentacorannulene CH as a strategy to produce CH as a precursor for C.. *RSC Advances*, **2020**, 10, 3689-3693	3.7	3
387	Reactivity of Cobalt-Fullerene Complexes towards Deuterium. *ChemPhysChem*, **2020**, 21, 1012-1018	3.2	3
386	Interaction of Hydrogen with Graphitic Surfaces, Clean and Doped with Metal Clusters **2020**, 545-566		
385	Nanoalloys of Metals Which Do Not Form Bulk Alloys: The Case of Ag-Co. *Journal of Physical Chemistry A*, **2020**, 124, 6468-6477	2.8	7
384	Cathodoluminescence in single and multiwall WS2 nanotubes: Evidence for quantum confinement and strain effect. *Applied Physics Reviews*, **2020**, 7, 041401	17.3	7
383	Dynamics of Cluster Isomerization Induced by Hydrogen Adsorption. *Journal of Physical Chemistry C* , **2019**, 123, 15236-15243	3.8	7
382	Hydrogen quenches the size effects in carbon clusters. *Physical Chemistry Chemical Physics*, **2019**, 21, 10402-10410	3.6	1
381	Bimetallic Al-Sn clusters: mixing at the nanoscale. *Physical Chemistry Chemical Physics*, **2019**, 21, 22919-22929	3.6	5
380	H2 Adsorption on Cu4-xMx (M = Au, Pt; x = 0□4) Clusters: Similarities and Differences As Predicted by Density Functional Theory. *Journal of Physical Chemistry C*, **2019**, 123, 30768-30780	3.8	6
379	Ab initio studies of ethanol dehydrogenation at binary AuPd nanocatalysts. *Molecular Catalysis*, **2018**, 449, 8-13	3.3	10
378	Modelling of adsorption and intercalation of hydrogen on/into tungsten disulphide multilayers and multiwall nanotubes. *Physical Chemistry Chemical Physics*, **2018**, 20, 12061-12074	3.6	2

377	Theoretical study of the adsorption of hydrogen on cobalt clusters. *Physical Chemistry Chemical Physics*, **2018**, 20, 21163-21176	3.6	15
376	Interaction of Hydrogen with Graphitic Surfaces, Clean and Doped with Metal Clusters **2018**, 1-22		
375	An improved descriptor of cluster stability: application to small carbon clusters. *Physical Chemistry Chemical Physics*, **2018**, 20, 27368-27374	3.6	8
374	Computer Simulations of the Structure of Nanoporous Carbons and Higher Density Phases of Carbon **2018**, 21-34		
373	Competition between Palladium Clusters and Hydrogen to Saturate Graphene Vacancies. *Journal of Physical Chemistry C*, **2017**, 121, 10843-10850	3.8	13
372	Steric and chemical effects on the hydrogen adsorption and dissociation on free and graphene□supported palladium clusters. *Computational and Theoretical Chemistry*, **2017**, 1107, 23-29	2	16
371	Hydrogen Chemical Configuration and Thermal Stability in Tungsten Disulfide Nanoparticles Exposed to Hydrogen Plasma. *Journal of Physical Chemistry C*, **2017**, 121, 11747-11756	3.8	4
370	Interaction of aromatic molecules with small gold clusters. *Chemical Physics Letters*, **2017**, 684, 91-96	2.5	7
369	Searching for DFT-based methods that include dispersion interactions to calculate the physisorption of H on benzene and graphene. *Journal of Chemical Physics*, **2017**, 146, 214104	3.9	20
368	Manipulating the Magnetic Moment of Palladium Clusters by Adsorption and Dissociation of Molecular Hydrogen. *Journal of Physical Chemistry C*, **2017**, 121, 20756-20762	3.8	8
367	Adsorption and growth of palladium clusters on graphdiyne. *Physical Chemistry Chemical Physics*, **2017**, 19, 19094-19102	3.6	30
366	Controlling the Adsorption of Carbon Monoxide on Platinum Clusters by Dopant-Induced Electronic Structure Modification. *Angewandte Chemie*, **2016**, 128, 11225-11229	3.6	22
365	The Diels-Alder Cycloaddition Reaction of Substituted Hemifullerenes with 1,3-Butadiene: Effect of Electron-Donating and Electron-Withdrawing Substituents. *Molecules*, **2016**, 21, 200	4.8	7
364	Controlling the Adsorption of Carbon Monoxide on Platinum Clusters by Dopant-Induced Electronic Structure Modification. *Angewandte Chemie - International Edition*, **2016**, 55, 11059-63	16.4	43
363	Is Spillover Relevant for Hydrogen Adsorption and Storage in Porous Carbons Doped with Palladium Nanoparticles?. *Journal of Physical Chemistry C*, **2016**, 120, 17357-17364	3.8	32
362	The diatomic dication SiC2+ in the gas phase. *Chemical Physics*, **2015**, 455, 41-47	2.3	1
361	Competition between molecular and dissociative adsorption of hydrogen on palladium clusters deposited on defective graphene. *RSC Advances*, **2015**, 5, 47945-47953	3.7	37
360	From graphene oxide to pristine graphene: revealing the inner workings of the full structural restoration. *Nanoscale*, **2015**, 7, 2374-90	7.7	83

359	Elimination vs substitution reaction. A dichotomy between Brønsted-Lowry and Lewis basicity. *Organic Letters*, **2015**, 17, 767-9	6.2	0
358	Metallicity enhancement in core–shell SiO2@RuO2 nanowires. *RSC Advances*, **2014**, 4, 34696-34700	3.7	1
357	Palladium Clusters Anchored on Graphene Vacancies and Their Effect on the Reversible Adsorption of Hydrogen. *Journal of Physical Chemistry C*, **2014**, 118, 5081-5090	3.8	60
356	Ab initio studies of propene epoxidation on oxidized silver surfaces. *Physical Chemistry Chemical Physics*, **2014**, 16, 26546-52	3.6	16
355	Tailoring structural and electronic properties of RuO2 nanotubes: a many-body approach and electronic transport. *Physical Chemistry Chemical Physics*, **2013**, 15, 14715-22	3.6	21
354	Protophilicity index and protofelicity equalization principle: new measures of Brønsted-Lowry-Lewis acid-base interactions. *Journal of Molecular Modeling*, **2013**, 19, 3961-7	2	2
353	Simulation of hydrogen storage in porous carbons. *Journal of Materials Research*, **2013**, 28, 589-604	2.5	28
352	Evolution of the atomic structure and the magnetism of small oxygen clusters. *Computational and Theoretical Chemistry*, **2013**, 1021, 215-221	2	2
351	Semiempirical fine-tuning for Hartree–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	2.3	3
350	Transport coefficients in the strongly coupled liquid alkali metals. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2013**, 377, 810-812	2.3	1
349	Electronic and magnetic properties of Fe clusters inside finite zigzag single-wall carbon nanotubes. *Physical Review B*, **2013**, 87,	3.3	7
348	Synthesis of fullerenes. *Journal of Physical Organic Chemistry*, **2013**, 26, 526-539	2.1	68
347	Comment on "The diatomic dication CuZn2+ in the gas phase" [J. Chem. Phys. 135, 034306 (2011)]. *Journal of Chemical Physics*, **2013**, 138, 077101	3.9	
346	Growth of fullerene fragments using the Diels-Alder cycloaddition reaction: first step towards a C60 synthesis by dimerization. *Molecules*, **2013**, 18, 2243-54	4.8	5
345	Ornstein–Zernike direct correlation function from diffraction experiments in supercooled liquid silicon and in disordered cobalt. *Physics and Chemistry of Liquids*, **2012**, 50, 131-136	1.5	
344	Adsorption and dissociation of molecular hydrogen on the edges of graphene nanoribbons. *Journal of Nanoparticle Research*, **2012**, 14, 1	2.3	12
343	First-Principles Structural and Electronic Characterization of Ordered SiO2 Nanowires. *Journal of Physical Chemistry C*, **2012**, 116, 18973-18982	3.8	20
342	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	

341	Adsorption and Dissociation of Molecular Hydrogen on Palladium Clusters Supported on Graphene. *Journal of Physical Chemistry C*, **2012**, 116, 21179-21189	3.8	86
340	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	2.3	34
339	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	1
338	Simulated porosity and electronic structure of nanoporous carbons. *Journal of Chemical Physics*, **2011**, 135, 104706	3.9	33
337	Simulation of the hydrogen storage in nanoporous carbons with different pore shapes. *International Journal of Hydrogen Energy*, **2011**, 36, 10748-10759	6.7	58
336	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	12
335	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	5.3	102
334	Surfactant effect of sulfuric acid on the exfoliation of bilayer graphene. *Physical Review B*, **2011**, 84,	3.3	12
333	The diatomic dication CuZn2+ in the gas phase. *Journal of Chemical Physics*, **2011**, 135, 034306	3.9	5
332	Structure and Properties of Atomic Nanoclusters **2011**,		15
331	Some properties of the structure factor S(q) in two-dimensional classical liquids near freezing. *Physics and Chemistry of Liquids*, **2010**, 48, 409-413	1.5	3
330	Lifetime of electronic excitations in metal nanoparticles. *New Journal of Physics*, **2010**, 12, 053023	2.9	13
329	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	3.9	35
328	Theoretical study of the transition from planar to three-dimensional structures of palladium clusters supported on graphene. *Physical Review B*, **2010**, 81,	3.3	110
327	Interaction of Surfactants Containing a Sulfuric Group with a (5,5) Carbon Nanotube. *Journal of Physical Chemistry C*, **2010**, 114, 17249-17256	3.8	8
326	High-pressure behaviour of crystalline silane compared with that for SnH4. *Phase Transitions*, **2009**, 82, 247-250	1.3	2
325	Fractal network dimension determining the relation between the strength of bulk metallic glasses and the glass transition temperature. *Applied Physics Letters*, **2009**, 95, 021909	3.4	5
324	Observation of Zr2(2+), Cd2(2+), Hf2(2+), W2(2+), and Pt2(2+) in the gas phase. *Journal of Chemical Physics*, **2009**, 130, 144312	3.9	13

323	Properties of glass-forming metallic liquids: when is there a hard-sphere-like behaviour?. *Physics and Chemistry of Liquids*, **2009**, 47, 585-598	1.5	1
322	Selective propene epoxidation on immobilized au(6-10) clusters: the effect of hydrogen and water on activity and selectivity. *Angewandte Chemie - International Edition*, **2009**, 48, 1467-71	16.4	224
321	New insights on the reaction mechanisms for CO oxidation on Au catalysts. *Chemical Physics Letters* , **2009**, 468, 201-204	2.5	17
320	Adsorption of Lithium on Finite Graphitic Clusters. *Journal of Physical Chemistry C*, **2009**, 113, 939-941	3.8	34
319	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	3.8	11
318	Transcending Lindemannıs 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	6
317	Half-metallic finite zigzag single-walled carbon nanotubes from first principles. *Physical Review B*, **2008**, 78,	3.3	42
316	Hydrogen storage capacities of nanoporous carbon calculated by density functional and MÏller-Plesset methods. *Physical Review B*, **2008**, 78,	3.3	46
315	Non-monotonic behaviour with concentration of the surface tension of certain binary liquid alloys. *Physics and Chemistry of Liquids*, **2008**, 46, 522-526	1.5	9
314	Interaction of narrow carbon nanotubes with nitronium tetrafluoroborate salts. *Journal of Chemical Physics*, **2008**, 128, 214703	3.9	5
313	Electronic and atomic structure of the Al(n)H(n+2) clusters. *Journal of Chemical Physics*, **2008**, 129, 074306	3.9	15
312	Shape of the hydrogen adsorption regions of MOF-5 and its impact on the hydrogen storage capacity. *Physical Review B*, **2008**, 78,	3.3	13
311	Mechanism of amorphisation in CuRu, a binary alloy with a positive heat of mixing. *Physics and Chemistry of Liquids*, **2008**, 46, 669-675	1.5	5
310	Hydrogen storage in pure and Li-doped carbon nanopores: combined effects of concavity and doping. *Journal of Chemical Physics*, **2008**, 128, 144704	3.9	50
309	Interaction and concerted diffusion of lithium in a (5,5) carbon nanotube. *Physical Review B*, **2008**, 78,	3.3	48
308	The interaction of sulfuric acid with graphene and formation of adsorbed crystals. *Nanotechnology*, **2007**, 18, 485705	3.4	27
307	Theoretical study of the photoabsorption spectrum of small chromium clusters. *Physical Review B*, **2007**, 76,	3.3	12
306	Interaction of the Charged Deuterium Cluster D3+ with Femtosecond Laser Pulses *Journal of Physical Chemistry C*, **2007**, 111, 17765-17772	3.8	14

305	The optimum average nanopore size for hydrogen storage in carbon nanoporous materials. *Carbon*, **2007**, 45, 2649-2658	10.4	149
304	Theoretical study of molecular hydrogen clusters. *European Physical Journal D*, **2007**, 43, 61-64	1.3	22
303	Long-Range van der Waals Interactions in Density Functional Theory. *Theoretical Chemistry Accounts*, **2007**, 117, 467-472	1.9	24
302	Ionization potentials of neutral atoms and positive ions in the limit of large atomic number. *Physical Review A*, **2007**, 75,	2.6	6
301	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,	2.6	13
300	Magnetic Properties of Atomic Clusters of the Transition Elements. *Reviews in Computational Chemistry*, **2007**, 191-248		0
299	Stability of silicon-doped C60 dimers. *Journal of Chemical Physics*, **2007**, 126, 044705	3.9	13
298	Chemical Properties of Small Au Clusters: An Analysis of the Local Site Reactivity. *Journal of Physical Chemistry C*, **2007**, 111, 6668-6677	3.8	68
297	Photoabsorption spectra of Ti8C12 metallocarbohedrynes: Theoretical spectroscopy within time-dependent density functional theory. *Journal of Chemical Physics*, **2006**, 125, 074311	3.9	14
296	Structural corrections to Stokes-Einstein relation for liquid metals near freezing. *Physical Review E*, **2006**, 73, 032201	2.4	9
295	Electrostrictive deformations in small carbon clusters, hydrocarbon molecules, and carbon nanotubes. *Physical Review A*, **2006**, 74,	2.6	4
294	Density functional calculations of hydrogen adsorption on boron nanotubes and boron sheets. *Nanotechnology*, **2006**, 17, 778-785	3.4	78
293	Density functional study of molecular hydrogen coverage on carbon nanotubes. *Computational Materials Science*, **2006**, 35, 238-242	3.2	50
292	Calculation of metastable free-energy diagrams and glass formation in the Mg□uY alloy and its boundary binaries using the Miedema model. *Intermetallics*, **2006**, 14, 297-307	3.5	31
291	Buckling in boron sheets and nanotubes. *Physica Status Solidi (A) Applications and Materials Science*, **2006**, 203, 1105-1110	1.6	22
290	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	0.3	8
289	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	0.3	5
288	Fragmentation and Coulomb explosion of deuterium clusters by the interaction with intense laser pulses. *Physical Review A*, **2005**, 72,	2.6	15

287	Simulating the thermal behavior and fragmentation mechanisms of exohedral and substitutional silicon-doped C60. *Journal of Chemical Physics*, **2005**, 123, 204323	3.9	31
286	Theoretical study of the reactivity of cesium with benzene and graphitic C(x)H(y) clusters. *Journal of Chemical Physics*, **2005**, 123, 074303	3.9	7
285	Enhancement of hydrogen physisorption on graphene and carbon nanotubes by Li doping. *Journal of Chemical Physics*, **2005**, 123, 204721	3.9	217
284	Structural and thermal stability of narrow and short carbon nanotubes and nanostrips. *Carbon*, **2005**, 43, 1371-1377	10.4	34
283	Adsorption of hydrogen on normal and pentaheptite single wall carbon nanotubes. *European Physical Journal D*, **2005**, 34, 279-282	1.3	23
282	A density-functional study on the formation of Mo(2)2+. *Journal of Chemical Physics*, **2005**, 123, 134313	3.9	5
281	BeB2 nanostructures: A density functional study. *Physical Review B*, **2005**, 72,	3.3	5
280	Charging mechanism for the bond elongation observed in suspended chains of gold atoms. *Physical Review B*, **2005**, 72,	3.3	12
279	Structure and Properties of Atomic Nanoclusters **2005**,		66
278	Deformations and thermal stability of carbon nanotube ropes. *IEEE Nanotechnology Magazine*, **2004** , 3, 230-236	2.6	21
277	Relativistic theory of an inhomogeneous electron liquid in relation to atomic binding energies. *Physics and Chemistry of Liquids*, **2004**, 42, 589-595	1.5	2
276	Excited states dynamics in time-dependent density functional theory. *European Physical Journal D*, **2004**, 28, 211-218	1.3	114
275	Calculation of the optical spectrum of the Ti8C12 and V8C12 Met-Cars. *Chemical Physics Letters*, **2004**, 398, 292-296	2.5	9
274	Interaction of molecular and atomic hydrogen with single-wall carbon nanotubes. *IEEE Nanotechnology Magazine*, **2004**, 3, 304-310	2.6	27
273	Interaction of lithium with graphene: An ab initio study. *Physical Review B*, **2004**, 70,	3.3	157
272	An Application of Non-Extensive Statistical Mechanics to Nanosystems. *Journal of Computational and Theoretical Nanoscience*, **2004**, 1, 227-229	0.3	40
271	Optical Properties of Nanostructures from Time-Dependent Density Functional Theory. *Journal of Computational and Theoretical Nanoscience*, **2004**, 1, 231-255	0.3	17
270	Coulomb explosion of deuterium cationic clusters. *Physical Review A*, **2003**, 68,	2.6	8

269	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	1.3	15
268	Growth Ability and Stability Indices of Clusters. *Journal of Cluster Science*, **2003**, 14, 31-47	3	7
267	Electronic metastable bound states of Mn22+ and Co22+. *Chemical Physics Letters*, **2003**, 372, 82-89	2.5	5
266	Metastable states in Au22+: a density functional study. *Computational and Theoretical Chemistry*, **2003**, 639, 203-211		3
265	Tight binding studies of exohedral silicon doped C60. *Composites Science and Technology*, **2003**, 63, 1499-1505	1.6	7
264	Structural and thermal properties of silicon-doped fullerenes. *Journal of Chemical Physics*, **2003**, 119, 1127-1135	3.9	37
263	Ab initio molecular dynamics simulations of the two-step melting of NaSn. *Physical Review B*, **2003**, 68,	3.3	1
262	Analysis of the bonding and reactivity of H and the Al13 cluster using density functional concepts. *Journal of Chemical Physics*, **2003**, 119, 5128-5141	3.9	53
261	Computer simulation of cluster assembling. *International Journal of Quantum Chemistry*, **2002**, 86, 226-238	1.1	17
260	Nonthermal fragmentation of C60. *Chemical Physics Letters*, **2002**, 352, 154-162	2.5	22
259	Patching and tearing single-wall carbon-nanotube ropes into multiwall carbon nanotubes. *Physical Review Letters*, **2002**, 89, 255501	7.4	44
258	Can optical spectroscopy directly elucidate the ground state of C20?. *Journal of Chemical Physics*, **2002**, 116, 1930-1933	3.9	51
257	Stability of a Sn4 tetrahedral cluster in an alkali atom environment. *Physical Review B*, **2002**, 65,	3.3	5
256	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	1.5	2
255	Conditions for the self-assembling of cluster materials. *Nanotechnology*, **2002**, 13, 253-257	3.4	22
254	Some Properties of a Model Liquid of C 60 Buckyballs. *Physics and Chemistry of Liquids*, **2002**, 40, 457-467	1.5	3
253	Interaction of molecular and atomic hydrogen with (5,5) and (6,6) single-wall carbon nanotubes. *Journal of Chemical Physics*, **2002**, 117, 2281-2288	3.9	184
252	Octet composition in alkali-Pb solid alloys. *Physical Review B*, **2002**, 66,	3.3	1

251	Metastable phase stability in the ternary ZrFeCr system. *Intermetallics*, **2002**, 10, 205-216	3.5	22
250	Amorphization in GdCo alloys and multilayers. *Journal of Physics Condensed Matter*, **2002**, 14, 8913-8924	1.8	15
249	ELECTRONIC SHELL EFFECTS IN METAL CLUSTERS AND THEIR CONSEQUENCES FOR CLUSTER SELF-ASSEMBLING **2002**, 1476-1507		2
248	Melting behavior of large disordered sodium clusters. *European Physical Journal D*, **2001**, 15, 221-227	1.3	27
247	Exchange energy density and some approximate exchange potentials obtained from HartreeFock theory of the ground state of the Be atom. *Chemical Physics Letters*, **2001**, 343, 166-170	2.5	6
246	Assembling of hydrogenated aluminum clusters. *European Physical Journal D*, **2001**, 16, 285-288	1.3	16
245	Novel polygonized single-wall carbon nanotube bundles. *Physical Review Letters*, **2001**, 86, 3056-9	7.4	107
244	Melting in Large Sodium Clusters: An Orbital-Free Molecular Dynamics Study. *Journal of Physical Chemistry B*, **2001**, 105, 2386-2392	3.4	52
243	Magnetic interactions between small Ni clusters. *Solid State Communications*, **2000**, 116, 309-314	1.6	
242	Theoretical evidence of bound metastable states in the doubly ionized nickel dimer Ni22+. *Chemical Physics Letters*, **2000**, 332, 481-486	2.5	7
241	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
240	Tight binding molecular dynamics studies of boron assisted nanotube growth. *Journal of Chemical Physics*, **2000**, 113, 3814-3821	3.9	34
239	Ab initio calculation of the lattice distortions induced by substitutional Ag and Cu impurities in alkali halide crystals. *Physical Review B*, **2000**, 62, 3086-3092	3.3	7
238	Computer simulation of the spreading of metallic clusters landing at grazing incidence on a metallic surface. *Physical Review B*, **2000**, 62, 16031-16039	3.3	8
237	Molecular dynamics study of cluster impact on the (001) and (110) surfaces of fcc metals. *Computational Materials Science*, **2000**, 17, 515-519	3.2	10
236	Density functional study of adsorption of molecular hydrogen on graphene layers. *Journal of Chemical Physics*, **2000**, 112, 8114-8119	3.9	229
235	Electronic and atomic structure, and magnetism of transition-metal clusters. *Chemical Reviews*, **2000**, 100, 637-78	68.1	451
234	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	1.3	8

233	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	1.5	19
232	Relation between transport and thermodynamic properties in liquid sp-electron metals near freezing. *Physical Review E*, **1999**, 60, 4125-9	2.4	8
231	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	3.3	55
230	Orbital-free molecular dynamics simulations of melting in Na8 and Na20: Melting in steps. *Journal of Chemical Physics*, **1999**, 111, 6026-6035	3.9	67
229	Ab initio study of B32 clusters: competition between spherical, quasiplanar and tubular isomers. *Chemical Physics Letters*, **1999**, 311, 21-28	2.5	99
228	Improved Charge Transfer at Carbon Nanotube Electrodes. *Advanced Materials*, **1999**, 11, 154-157	24	435
227	Simulating the thermal stability and phase changes of small carbon clusters and fullerenes. *European Physical Journal D*, **1999**, 6, 221-233	1.3	24
226	Assembling alkali□lead solid compounds from clusters. *Journal of Chemical Physics*, **1999**, 111, 7053-7061	3.9	8
225	Magnetic moments of. *European Physical Journal D*, **1999**, 6, 235	1.3	15
224	Electronic Structure of Bimetallic Clusters Based on Alkali Elements. *Springer Series in Cluster Physics*, **1999**, 255-276		
223	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	2.5	15
222	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	2.5	1
221	Comparative ab initio studies of small tin and lead clusters. *Annalen Der Physik*, **1998**, 510, 107-119	2.6	8
220	Mixed lead□alkali clusters in the gas phase and in liquid alloys. *International Journal of Quantum Chemistry*, **1998**, 69, 341-348	2.1	3
219	Building alkali-lead intermetallic compounds from clusters. *Solid State Communications*, **1998**, 108, 519-524	2.6	8
218	Lattice distortions around a Tl+ impurity in NaI:Tl+ and CsI:Tl+ scintillators: An ab initio study involving large active clusters. *Physical Review B*, **1998**, 58, 11964-11969	3.3	13
217	Structure, transport and surface properties of dense fluids, especially liquid metals. *Molecular Physics*, **1998**, 95, 353-361	1.7	7
216	Magnetic moments of Ni clusters. *Physical Review B*, **1998**, 57, 12469-12475	3.3	67

215	Ab initio calculations of structures and stabilities of (NaI)nNa+ and (CsI)nCs+ cluster ions. *Physical Review B*, **1998**, 58, 9972-9979	3.3	34
214	Comparative ab initio studies of small tin and lead clusters. *Annalen Der Physik*, **1998**, 7, 107-119	2.6	34
213	Theoretical Study of the Collective Electronic Excitations of the Endohedral Clusters NaN@C780 **1998**, 133-141		
212	Ab initio study of (NaCl)nNA+ clusters. *Canadian Journal of Physics*, **1998**, 76, 311-320	1.1	3
211	Theoretical Study of the Metal-Nonmetal Transition in Transition Metal Clusters **1998**, 109-117		1
210	Geometrical effects on the magnetism of small Ni clusters. *Physical Review B*, **1997**, 55, 13279-13282	3.3	47
209	Clusters and layers of C60 molecules supported on a graphite substrate. *Physical Review B*, **1997**, 55, 7190-7197	3.3	42
208	Theoretical Models for the Optical Properties of Clusters and Nanostructures. *International Journal of Modern Physics B*, **1997**, 11, 2727-2776	1.1	23
207	Theoretical Study of Small (NaI)nClusters. *Journal of Physical Chemistry B*, **1997**, 101, 5944-5950	3.4	24
206	Structure and bonding in small neutral alkali halide clusters. *Physical Review B*, **1997**, 56, 15353-15360	3.3	60
205	Thermal behaviour of carbon clusters and small fullerenes. *Zeitschrift F□ Physik D-Atoms Molecules and Clusters*, **1997**, 40, 385-388		6
204	Density functional pseudopotential study of the endohedral complex Li2@C60. *Physica B: Condensed Matter*, **1997**, 240, 154-166	2.8	2
203	Nonmetal-metal transition in Ni clusters. *Solid State Communications*, **1997**, 104, 635-639	1.6	17
202	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	1.3	1
201	Study of clusters of interest for liquid ionic alloys. *Annalen Der Physik*, **1997**, 509, 35-44	2.6	6
200	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	2.1	3
199	Ionic vibrational breathing mode of metallic clusters. *International Journal of Quantum Chemistry*, **1997**, 61, 613-626	2.1	5
198	Thermal road for fullerene annealing. *Chemical Physics Letters*, **1997**, 273, 367-370	2.5	27

197	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	1.3	10
196	Density functional theory of clusters of nontransition metals using simple models. *Topics in Current Chemistry*, **1996**, 119-171		6
195	Theoretical study of icosahedral Ni clusters within the embedded-atom method. *Physical Review B*, **1996**, 54, 5961-5969	3.3	45
194	Structural and dynamical properties of CuAu bimetallic clusters. *Journal of Chemical Physics*, **1996**, 104, 1056-1066	3.9	111
193	Ab Initio Photoabsorption Spectra and Structures of Small Semiconductor and Metal Clusters. *Physical Review Letters*, **1996**, 77, 247-250	7.4	156
192	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
191	Clusters of Fullerene Molecules. *Materials Science Forum*, **1996**, 232, 155-172	0.4	
190	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	4.3	8
189	Theoretical study of the binding of Na clusters encapsulated in the C240 fullerene. *Physical Review B*, **1996**, 53, 16059-16066	3.3	19
188	Tight-binding study of the ionization of iron clusters. *Physical Review B*, **1996**, 54, 3003-3006	3.3	21
187	Theoretical study of gas-phase NanPb clusters and implications for liquid NaPb alloys. *Journal of Chemical Physics*, **1996**, 104, 8043-8047	3.9	8
186	ON THE FISSION OF CHARGED ALKALI-METAL CLUSTERS. *Surface Review and Letters*, **1996**, 03, 617-621	1.1	3
185	Semi-empirical model for the fission of multiply charged metal clusters. *Zeitschrift Für Physik D-Atoms Molecules and Clusters*, **1995**, 33, 301-305		4
184	An experimental and theoretical study of the glass-forming region of the Mg-Cu-Sn system. *Journal of Materials Science*, **1995**, 30, 40-46	4.3	12
183	Thermodynamic analysis of irradiation-induced amorphization of intermetallic particles in Zircaloy. *Journal of Materials Science*, **1995**, 30, 196-200	4.3	9
182	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	2.1	2
181	Vibrational frequencies of sodium clusters. *International Journal of Quantum Chemistry*, **1995**, 56, 589-601	2.1	6
180	Density functional theory of the collective electronic excitations in NanKn clusters. *International Journal of Quantum Chemistry*, **1995**, 56, 839-846	2.1	6

179	Exchange and correlation in density functional theory. *International Journal of Quantum Chemistry*, **1995**, 56, 49-59	2.1	10
178	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	2.3	7
177	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	1.6	2
176	Charge transfer within zintl ions in liquid metallic alloys. A cluster study. *Computational and Theoretical Chemistry*, **1995**, 330, 267-272		7
175	Deformed-jellium model for the fission of multiply charged simple metal clusters. *Physical Review B* , **1995**, 51, 1897-1901	3.3	14
174	Theoretical study of the collective electronic excitations in single- and multiple-shell fullerenes. *Physical Review B*, **1995**, 52, 8446-8453	3.3	7
173	Screening of an Ion in a Finite Electron Gas and its Relation to Cluster Structure. *Physics and Chemistry of Liquids*, **1995**, 29, 23-30	1.5	1
172	Theoretical study of (NaCl)n clusters. *Physica B: Condensed Matter*, **1995**, 212, 329-342	2.8	18
171	Fission barriers for Na N 2+ cluster dissociation **1995**, 231-234		
170	Symmetric and asymmetric fission of charged sodium clusters. *Acta Physica Hungarica A Heavy Ion Physics*, **1995**, 1, 227-240		
169	Molecular-dynamics study of the structure, binding energy, and melting of small clusters of fullerene molecules using Girifalcols spherical model. *Physical Review B*, **1994**, 49, 8491-8494	3.3	52
168	Barrier for the reaction X20++X20+-->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	3.3	8
167	Collective electronic excitations in metal-coated C60. *Physical Review B*, **1994**, 49, 17397-17402	3.3	13
166	Atomic and electronic structure of Na10K10Cs n clusters. *Zeitschrift F Physik D-Atoms Molecules and Clusters*, **1994**, 30, 349-356		6
165	Fission barriers for Na 2+ N cluster dissociation. *Zeitschrift F Physik D-Atoms Molecules and Clusters*, **1994**, 31, 275-277		6
164	Molecular dynamics study of A18B lennard-jones clusters. *Zeitschrift F Physik D-Atoms Molecules and Clusters*, **1994**, 31, 299-301		3
163	Nonlocal exchange and kinetic energy density functionals with correct asymptotic behavior for electronic systems. *International Journal of Quantum Chemistry*, **1994**, 49, 171-184	2.1	18
162	Ionization potentials of atoms calculated with a nonlocal exchange and a local correlation functional. *International Journal of Quantum Chemistry*, **1994**, 52, 993-1010	2.1	9

161	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	18
160	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	3.3	91
159	Embedded-atom method applied to bimetallic clusters: The Cu-Ni and Cu-Pd systems. *Physical Review B*, **1994**, 49, 16649-16658	3.3	44
158	Density functional theory of the structure of bimetallic clusters. *Physica Scripta*, **1994**, T55, 177-182	2.6	6
157	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		11
156	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		8
155	Density approximation to the average Hartree-Fock exchange potential for atoms. *Journal of Chemical Sciences*, **1994**, 106, 91-102	1.8	
154	Molecular-dynamics study of the binding energy and melting of transition-metal clusters. *Physical Review B*, **1993**, 48, 8253-8262	3.3	122
153	Potential energy curve of H+ 2 related to mirror-plane ground-state electron density. *Molecular Physics*, **1993**, 79, 1143-1146	1.7	5
152	Dissociation energy of alkali metal clusters related to inhomogeneous electron gas theory. *Molecular Physics*, **1993**, 79, 393-403	1.7	12
151	A theoretical study of the static structure and thermodynamics of liquid lithium. *Journal of Physics Condensed Matter*, **1993**, 5, 4283-4298	1.8	41
150	Charge transfer within clusters in liquid ionic alloys. *Journal of Physics Condensed Matter*, **1993**, 5, 4271-4282		4
149	Nonlocal exchange- and kinetic-energy density functionals for electronic systems: Application to atoms and ions. *Physical Review A*, **1993**, 47, 1804-1810	2.6	13
148	Self-consistent local-density approximation with model Coulomb pair-correlation functions for electronic systems. *Physical Review A*, **1993**, 47, 1811-1816	2.6	14
147	Stabilities of large sodium clusters for different atomic arrangements. *Physical Review B*, **1993**, 47, 4747-4755	3.3	9
146	Weighted-density exchange and local-density Coulomb correlation energy functionals for finite systems: Application to atoms. *Physical Review A*, **1993**, 48, 4197-4212	2.6	39
145	Hardness of metallic clusters **1993**, 229-257		2
144	Non-local exchange and local Coulomb correlation energy density functionals for finite many-electron systems. *Chemical Physics Letters*, **1993**, 205, 348-353	2.5	19

143	Surface plasmon excitations in C60, C60K and C60H clusters. *Physica B: Condensed Matter*, **1993**, 183, 247-263	2.8	28
142	Nonlocal approximation to the exchange and kinetic energy functionals: Application to metallic clusters. *International Journal of Quantum Chemistry*, **1993**, 45, 333-347	2.1	9
141	Theoretical study of NaCl clusters. *Zeitschrift F Physik D-Atoms Molecules and Clusters*, **1993**, 26, 213-215		14
140	Photoabsorption cross sections of sodium clusters: electronic and geometrical effects. *Zeitschrift F Physik D-Atoms Molecules and Clusters*, **1993**, 26, 284-286		5
139	Atomic structure and collective excitations of medium size NanKm clusters. *Zeitschrift F Physik D-Atoms Molecules and Clusters*, **1993**, 28, 311-319		10
138	Glass formation in the Cu Ti 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		10
137	Atomic structure of metallic clusters of medium size. *International Journal of Modern Physics B*, **1992**, 06, 3613-3621	1.1	
136	Theoretical study of the photoabsorption spectrum of Na8, Na20, Cs8, and Cs10O clusters. *Physical Review B*, **1992**, 45, 13657-13663	3.3	34
135	Influence of nonlocal exchange-correlation effects on the response properties of simple metal clusters. *Physical Review B*, **1992**, 46, 4891-4898	3.3	46
134	Electronic and atomic structure of simple-metal clusters: Beyond the spherical jellium model **1992**, 327-334		4
133	Nonlocal exchange and kinetic-energy density functionals for electronic systems. *International Journal of Quantum Chemistry*, **1992**, 44, 347-358	2.1	9
132	Theoretical calculation of the amorphous alloy range of the Mg-Cu system. *Journal of Materials Science*, **1992**, 27, 4935-4939	4.3	9
131	A molecular dynamics study of the evaporation of small argon clusters. *Physica B: Condensed Matter* , **1992**, 179, 273-277	2.8	21
130	Distribution of interatomic distances in large metallic clusters. *Zeitschrift F Physik D-Atoms Molecules and Clusters*, **1992**, 22, 541-545		12
129	Dissociation of doubly charged alkali metal clusters. *Annalen Der Physik*, **1992**, 504, 270-280	2.6	17
128	Dissociation of doubly-charged alkali-metal clusters **1992**, 112-117		
127	Fragmentation of Doubly Charged Alkali-Metal Clusters. *Springer Series in Nuclear and Particle Physics*, **1992**, 305-311		2
126	Prediction of Metastable Alloy Formation and Phase Transformations Induced by Ion Bombardment in Binary Metal Systems **1992**, 328-335		2

125	Electronic structure of negatively charged aluminium clusters. *Physica B: Condensed Matter*, **1991**, 168, 32-38	2.8	15
124	Evaporation rates of hot sodium clusters. *Zeitschrift F Physik D-Atoms Molecules and Clusters*, **1991**, 20, 119-122		3
123	Response properties of sodium clusters within a jellium-like model with finite surface thickness. *Zeitschrift F Physik D-Atoms Molecules and Clusters*, **1991**, 19, 93-96		42
122	Stability of isomeric Na n clusters. *Zeitschrift F Physik D-Atoms Molecules and Clusters*, **1991**, 19, 141-143		6
121	One-Electron Energy Eigenvalues in the Weighted-Density Approximation to Exchange and Correlation. *Europhysics Letters*, **1991**, 14, 323-329	1.6	15
120	Coulomb barriers in the dissociation of doubly charged clusters. *Physical Review B*, **1991**, 43, 9459-9466	3.3	39
119	Inhomogeneous contraction of interatomic distances in metallic clusters: Calculations for Csn and OCsn. *Physical Review B*, **1991**, 44, 7273-7282	3.3	18
118	Evaporation rates of hot sodium clusters **1991**, 569-572		
117	Electronic and Atomic Structure of NanZn Clusters in the Spherically Averaged Pseudopotential Model **1991**, 373-386		2
116	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		89
115	Electronic and atomic structure of Cs N and Cs N O clusters. *Zeitschrift F Physik D-Atoms Molecules and Clusters*, **1990**, 17, 203-208		8
114	Density functional study of neutral and charged sodium and lead clusters in the jellium model. *Physica B: Condensed Matter*, **1990**, 167, 19-32	2.8	19
113	Polarizabilities of aluminium clusters. *Solid State Communications*, **1990**, 75, 139-142	1.6	15
112	Atomic structure and segregation in alkali-metal heteroclusters. *Physical Review B*, **1990**, 42, 5000-5008	3.3	26
111	Dissociation channels of NaN+ clusters (3 . *Physical Review B*, **1990**, 41, 5595-5601	3.3	22
110	Structure and energetics of Nan-xLix (n . *Physical Review B*, **1990**, 41, 5636-5642	3.3	20
109	Glass formation in ternary transition metal alloys. *Journal of Physics Condensed Matter*, **1990**, 2, 6245-6250	1.8	73
108	Surface Thickness of Liquid Metals Related to Surface Energy and Bulk Compressibility: A Universal Relation. *Physics and Chemistry of Liquids*, **1990**, 21, 257-259	1.5	7

107	PREDICTION OF GLASS FORMATION BY SOLID STATE REACTION IN ALLOYS. *Journal De Physique Colloque*, **1990**, 51, C4-111-C4-117		2
106	Vacancy Formation Energy in Close-packed Metals Connected with Liquid Thermodynamics at Melting. *Physics and Chemistry of Liquids*, **1989**, 20, 235-240	1.5	3
105	Coulomb explosion of charged jellium clusters. *Zeitschrift F Physik D-Atoms Molecules and Clusters* , **1989**, 11, 323-326		13
104	Enrichment and segregation in alkali heteroclusters. *Zeitschrift F Physik D-Atoms Molecules and Clusters*, **1989**, 12, 237-239		7
103	Immersion of hydrogen atoms in aluminium clusters. *Zeitschrift F Physik D-Atoms Molecules and Clusters*, **1989**, 13, 269-275		18
102	Possibility of spontaneous vitrification in Ti-Cr alloys. *Physica B: Condensed Matter*, **1989**, 160, 108-112	2.8	10
101	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	2.3	5
100	Electronic structure of CsN and CsNO clusters. *Solid State Communications*, **1989**, 71, 591-594	1.6	14
99	Enrichment and segregation in alkali heteroclusters **1989**, 237-239		
98	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		2
97	Theoretical study of the stability of AgN2+, AgN, AgN, AgN and NaN clusters as a function of size using the density functional formalism. *Chemical Physics*, **1988**, 120, 239-247	2.3	34
96	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	3.9	14
95	Stability and magic numbers of hetero-atomic clusters of simple metals. *Physica B: Condensed Matter*, **1988**, 154, 73-81	2.8	54
94	Determination of phase diagrams of eutectic binary alloys with partial solid solubility. *Physica B: Condensed Matter*, **1988**, 154, 82-86	2.8	5
93	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		1
92	Electronic and atomic structure of Na, Mg, Al and Pb clusters. *Zeitschrift F Physik D-Atoms Molecules and Clusters*, **1988**, 11, 163-174		83
91	Correlation of Glass Forming Ability with Thermochemical Coordinates*. *Zeitschrift Fur Physikalische Chemie*, **1988**, 156, 109-113	3.1	4
90	Size effects on the vacancy-formation energy of small sodium clusters in the jellium model. *Physical Review B*, **1988**, 37, 8436-8439	3.3	5

89	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		50
88	Prediction of the glass formation range of transition metal alloys. *Journal of Physics F: Metal Physics* , **1988**, 18, 2149-2157		45
87	On the Concentration Dependence of the Ordering Potential in Liquid Li-Pb Alloys. *Physics and Chemistry of Liquids*, **1987**, 16, 249-258	1.5	11
86	Simple density functional theory of the electronegativity and other related properties of atoms and ions **1987**, 41-78		6
85	Stability and magic numbers of small KxMg clusters. *Journal of Physics F: Metal Physics*, **1987**, 17, L197-L200		11
84	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	3.3	126
83	Surface Energy of Liquid Transition Metals Related to Bulk Compressibility and Thickness. *Physics and Chemistry of Liquids*, **1987**, 17, 209-214	1.5	9
82	A non local density functional calculation of the diamagnetic susceptibilities and other electronic properties of noble gases and closed-shell ions. *Zeitschrift F□ Physik D-Atoms Molecules and Clusters*, **1987**, 6, 219-226		8
81	Density Functional Calculation of the Fragmentation of Neutral, Singly and Doubly-Ionized Spherical Jellium-Like Metallic Microparticles **1987**, 263-267		
80	Nonlocal density functional calculation of the electron affinity of atoms. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **1986**, 114, 236-240	2.3	12
79	A hard-sphere description of the thermodynamic properties of binary mixtures of organic molecules. *Chemical Physics*, **1986**, 103, 35-42	2.3	4
78	Electron density and atomic relaxation around a vacancy in a small metal particle. *Zeitschrift F□ Physik D-Atoms Molecules and Clusters*, **1986**, 2, 177-181		3
77	Density functional theory of the chemical potential of atoms and its relation to electrostatic potentials and bonding distances. *Zeitschrift F□ Physik D-Atoms Molecules and Clusters*, **1986**, 1, 215-221		5
76	Magic numbers of sodium clusters. *Solid State Communications*, **1986**, 57, 85-88	1.6	30
75	Density-functional calculation of the fragmentation of doubly ionized spherical jelliumlike metallic microparticles. *Physical Review B*, **1986**, 34, 2152-2157	3.3	46
74	Asymmetric rare gas pair potentials from energy density functionals. *Journal of Chemical Physics*, **1986**, 85, 6637-6644	3.9	2
73	Glass-forming ability in binary alloys produced by ion beam mixing and by laser quenching. *Materials Letters*, **1986**, 4, 316-319	3.3	43
72	Local behavior of the kinetic energy in density functional theory. *International Journal of Quantum Chemistry*, **1985**, 27, 393-406	2.1	12

71	Density Functional Pseudopotential Calculation of the Cohesive Properties of Disordered Solid Alloys of Alkaline-Earth Metals. Influence of the Ionic Pseudopotential. *Physica Status Solidi (B): Basic Research*, **1985**, 129, 483-488	1.3	2
70	Liquidus Curves of Eutectic Na?K and Na?Cs Systems from Semiempirical Theories of Mixtures. *Physica Status Solidi A*, **1985**, 89, 73-78		2
69	Electronic and elastic effects in the interaction of impurities in ternary metallic alloys. *Journal of Physics and Chemistry of Solids*, **1985**, 46, 1147-1151	3.9	10
68	Density functional calculation of the ionization potentials of small metallic particles. *European Physical Journal B*, **1985**, 59, 187-191	1.2	8
67	Theory of the thermodynamic properties of binary mixtures of organic molecules with size mismatch. *Chemical Physics*, **1985**, 99, 35-41	2.3	10
66	Semiempirical Theory of Solid Solubility in Transition Metal Alloys. *Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences*, **1985**, 40, 1199-1205	1.4	48
65	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		5
64	Concentration Fluctuations in Binary Mixtures of Inert-Gas Fluids. *Physics and Chemistry of Liquids*, **1985**, 15, 41-48	1.5	2
63	Surface energy of liquid metals at the melting temperature related to bulk liquid structure. *Surface Science*, **1985**, 160, 509-516	1.8	26
62	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	1.4	
61	Liquidus Curves of Eutectic NaK and NaCs Systems. *Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences*, **1984**, 39, 842-845	1.4	4
60	Cohesive energy of small metallic particles. *Solid State Communications*, **1984**, 50, 549-552	1.6	10
59	Density functional calculation of the electronegativity and other related properties of atoms and ions of the principal groups of the periodic table. *Zeitschrift F□ Physik A*, **1984**, 319, 275-282		5
58	On the chemical potential of atomic ions. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **1984**, 101, 20-22	2.3	5
57	Role of the Excess Volume of Formation on Alloying. *Physica Status Solidi (B): Basic Research*, **1984**, 123, 485-489	1.3	4
56	On the Factors Controlling Glass Forming Ability of Metallic Alloys Formed by Fast Liquid Quenching. *Physica Status Solidi A*, **1984**, 81, 55-61		33
55	The Atomic Size-Mismatch Contribution to the Enthalpy of Formation of Concentrated Substitutional Metallic Solid Solutions. *Physica Status Solidi A*, **1984**, 85, 423-428		32
54	Relation between total energy, electronic potential at the nucleus, and chemical potential of positive ions. *International Journal of Quantum Chemistry*, **1984**, 26, 145-149	2.1	3

53	Concentration Fluctuations in Liquid Sodium-Caesium Alloys. *Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences*, **1984**, 39, 596-599	1.4	2
52	Semiempirical theory of solid solubility in metallic alloys. *Physica Status Solidi A*, **1983**, 76, 675-682		15
51	Density functional pseudopotential calculation of the cohesive properties of disordered solid alloys of nontransition metals application to ZnCd. *Physica Status Solidi (B): Basic Research*, **1983**, 119, 589-594	1.3	5
50	Density functional estimates of charge transfer and chemical potentials in hydrogen halides and mixed halides. *Chemical Physics*, **1983**, 76, 121-124	2.3	6
49	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		6
48	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	2.3	2
47	Prediction of amorphous alloy formation by ion beam mixing. *Solid State Communications*, **1983**, 48, 765-767	1.7	101
46	Electronegativity equalization and electron transfer in molecules. *Molecular Physics*, **1983**, 48, 981-988	1.7	9
45	Electronic and cohesive properties of small sodium particles. *Surface Science*, **1983**, 127, 367-376	1.8	21
44	Density functional theory of asymptotic form of electron density in heteronuclear diatomic molecules. *Journal of Chemical Physics*, **1983**, 79, 1903-1905	3.9	4
43	Equivalence of ionization potential and magnitude of chemical potential in Hartree-Fock theory of atoms. *Journal of Chemical Physics*, **1983**, 78, 1382-1383	3.9	28
42	On the free energy of mixing of a binary liquid alloy. *Physics and Chemistry of Liquids*, **1983**, 12, 265-268	1.5	1
41	Simple charge transfer model of X-ray scattering by ten-electron molecules. *Molecular Physics*, **1983**, 50, 789-796	1.7	7
40	Charge transfer in simple metallic alloys. *Journal De Physique*, **1983**, 44, 229-234		12
39	Electronegativity of fractionally charged atoms in the Density Functional Theory. *Zeitschrift Für Physik A*, **1983**, 312, 95-98		6
38	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		15
37	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		15
36	Electronegativity of positive ions in the density functional theory. *Zeitschrift Für Physik A*, **1982**, 305, 31-37		17

35	Prediction of solid solubility in alloys. Application to noble metal based alloys. *Acta Metallurgica*, **1982**, 30, 105-107		21
34	Concentration fluctuations in simple metallic liquid alloys. *Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics*, **1982**, 114, 67-70		5
33	Simple model for liquid metal alloys and relation to Miedemals variables. *Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics*, **1982**, 114, 141-146		
32	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		2
31	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		1
30	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		4
29	Semiempirical Study of Metastable Alloys Obtained by Ion Implantation in Metals and Semiconductors. *Physica Status Solidi A*, **1982**, 72, 777-781		6
28	Cellular density functional theory of the heat of formation of disordered simple alloys. *Physica Status Solidi (B): Basic Research*, **1982**, 114, 495-501	1.3	3
27	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	2.1	8
26	Relation of Regular Solution Theory of Liquid Metal Alloys to Miedemals Work. *Physics and Chemistry of Liquids*, **1981**, 11, 135-139	1.5	4
25	Density Functional theory of the atomic electronegativity. *Zeitschrift F□ Physik A*, **1981**, 302, 307-310		11
24	Volume Dependence of the Bulk Modulus in Alkali Metals. *Physica Status Solidi (B): Basic Research*, **1981**, 104, 307-312	1.3	11
23	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		3
22	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	2.3	11
21	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	2.3	3
20	Surface dipole barrier in metals. Relation to the bulk electron density. *Zeitschrift F□ Physik B Condensed Matter and Quanta*, **1981**, 40, 307-309		4
19	Density functional-pseudopotential approach to the heat of formation in alloys of alkali metals. *Journal of Physics F: Metal Physics*, **1981**, 11, 2045-2053		15
18	Partial Pressure Contributions to the Equation of State of Alkali Metals. *Physica Status Solidi (B): Basic Research*, **1980**, 100, 701-704	1.3	12

17	Semiempirical calculation of the surface dipole barrier in metals. *Solid State Communications*, **1980**, 33, 59-62	1.6	12
16	A theory of order-Disorder and antiphase domain boundary energies. *Metallurgical and Materials Transactions A - Physical Metallurgy and Materials Science*, **1980**, 11, 1747-1753		10
15	Electron density in simple metals. Relation to bulk and surface properties. *Journal of Physics F: Metal Physics*, **1980**, 10, 1995-2008		16
14	Prediction of solid solubility in alloys. *Physical Review B*, **1980**, 22, 5583-5589	3.3	68
13	Atomic electronegativity from density functional theory. *Journal of Chemical Physics*, **1980**, 73, 1313-1319	3.9	21
12	Volume of formation and electronic configuration in dilute alloys. *Journal of Physics and Chemistry of Solids*, **1979**, 40, 449-455	3.9	15
11	On the electronegativity parameters of the theory of heats of alloy formation. *Solid State Communications*, **1979**, 31, 9-14	1.6	19
10	Electronegativity scale for metals. *Physical Review B*, **1979**, 19, 3889-3895	3.3	45
9	Charge transfer and heat of formation in CsCl intermetallic compounds. *Journal of Physics and Chemistry of Solids*, **1978**, 39, 79-87	3.9	39
8	Gradient corrections in the energy density functional. *Chemical Physics Letters*, **1978**, 53, 190-191	2.5	21
7	Nonlocality and the energy of alloy formation. *Journal of Physics F: Metal Physics*, **1978**, 8, 2455-2460		39
6	Nonlocal approximation to the exchange potential and kinetic energy of an inhomogeneous electron gas. *Physical Review B*, **1978**, 17, 3735-3743	3.3	275
5	A non-local approximation to the exchange energy of the non-homogeneous electron gas. *Solid State Communications*, **1977**, 24, 135-138	1.6	87
4	Charge transfer in binary alloys and to impurities in iron. *Journal of Physics and Chemistry of Solids*, **1977**, 38, 869-876	3.9	22
3	Semi-statistical model for metals. *Journal of Physics and Chemistry of Solids*, **1977**, 38, 307-310	3.9	11
2	On the derivation of the Schrödinger equation from Newtonian mechanics. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **1972**, 38, 501-502	2.3	1
1	Structure, stability, and optical absorption spectra of small TinCx clusters: a first-principles approach. *Monthly Notices of the Royal Astronomical Society*,	4.3	1