Julio A Alonso

List of Publications by Citations

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	Electronic and atomic structure, and magnetism of transition-metal clusters. *Chemical Reviews*, **2000**, 100, 637-78	68.1	451
393	Improved Charge Transfer at Carbon Nanotube Electrodes. *Advanced Materials*, **1999**, 11, 154-157	24	435
392	Nonlocal approximation to the exchange potential and kinetic energy of an inhomogeneous electron gas. *Physical Review B*, **1978**, 17, 3735-3743	3.3	275
391	Density functional study of adsorption of molecular hydrogen on graphene layers. *Journal of Chemical Physics*, **2000**, 112, 8114-8119	3.9	229
390	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
389	Enhancement of hydrogen physisorption on graphene and carbon nanotubes by Li doping. *Journal of Chemical Physics*, **2005**, 123, 204721	3.9	217
388	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
387	Interaction of lithium with graphene: An ab initio study. *Physical Review B*, **2004**, 70,	3.3	157
386	Ab Initio Photoabsorption Spectra and Structures of Small Semiconductor and Metal Clusters. *Physical Review Letters*, **1996**, 77, 247-250	7.4	156
385	The optimum average nanopore size for hydrogen storage in carbon nanoporous materials. *Carbon*, **2007**, 45, 2649-2658	10.4	149
384	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
383	Molecular-dynamics study of the binding energy and melting of transition-metal clusters. *Physical Review B*, **1993**, 48, 8253-8262	3.3	122
382	Excited states dynamics in time-dependent density functional theory. *European Physical Journal D*, **2004**, 28, 211-218	1.3	114
381	Structural and dynamical properties of Cu$_n$Au bimetallic clusters. *Journal of Chemical Physics*, **1996**, 104, 1056-1066	3.9	111
380	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
379	Novel polygonized single-wall carbon nanotube bundles. *Physical Review Letters*, **2001**, 86, 3056-9	7.4	107
378	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

377	Prediction of amorphous alloy formation by ion beam mixing. *Solid State Communications*, **1983**, 48, 765-767	1.67	101
376	Ab initio study of B32 clusters: competition between spherical, quasiplanar and tubular isomers. *Chemical Physics Letters*, **1999**, 311, 21-28	2.5	99
375	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
374	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
373	A non-local approximation to the exchange energy of the non-homogeneous electron gas. *Solid State Communications*, **1977**, 24, 135-138	1.6	87
372	Adsorption and Dissociation of Molecular Hydrogen on Palladium Clusters Supported on Graphene. *Journal of Physical Chemistry C*, **2012**, 116, 21179-21189	3.8	86
371	From graphene oxide to pristine graphene: revealing the inner workings of the full structural restoration. *Nanoscale*, **2015**, 7, 2374-90	7.7	83
370	Electronic and atomic structure of Na, Mg, Al and Pb clusters. *Zeitschrift F□ Physik D-Atoms Molecules and Clusters*, **1988**, 11, 163-174		83
369	Density functional calculations of hydrogen adsorption on boron nanotubes and boron sheets. *Nanotechnology*, **2006**, 17, 778-785	3.4	78
368	Glass formation in ternary transition metal alloys. *Journal of Physics Condensed Matter*, **1990**, 2, 6245-6250	2.8	73
367	Synthesis of fullerenes. *Journal of Physical Organic Chemistry*, **2013**, 26, 526-539	2.1	68
366	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
365	Prediction of solid solubility in alloys. *Physical Review B*, **1980**, 22, 5583-5589	3.3	68
364	Magnetic moments of Ni clusters. *Physical Review B*, **1998**, 57, 12469-12475	3.3	67
363	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
362	Structure and Properties of Atomic Nanoclusters **2005**,		66
361	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
360	Structure and bonding in small neutral alkali halide clusters. *Physical Review B*, **1997**, 56, 15353-15360	3.3	60

359	Simulation of the hydrogen storage in nanoporous carbons with different pore shapes. *International Journal of Hydrogen Energy*, **2011**, 36, 10748-10759	6.7	58
358	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
357	Stability and magic numbers of hetero-atomic clusters of simple metals. *Physica B: Condensed Matter*, **1988**, 154, 73-81	2.8	54
356	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
355	Melting in Large Sodium Clusters: An Orbital-Free Molecular Dynamics Study. *Journal of Physical Chemistry B*, **2001**, 105, 2386-2392	3.4	52
354	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
353	Can optical spectroscopy directly elucidate the ground state of C20?. *Journal of Chemical Physics*, **2002**, 116, 1930-1933	3.9	51
352	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
351	Density functional study of molecular hydrogen coverage on carbon nanotubes. *Computational Materials Science*, **2006**, 35, 238-242	3.2	50
350	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
349	Interaction and concerted diffusion of lithium in a (5,5) carbon nanotube. *Physical Review B*, **2008**, 78,	3.3	48
348	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
347	Geometrical effects on the magnetism of small Ni clusters. *Physical Review B*, **1997**, 55, 13279-13282	3.3	47
346	Hydrogen storage capacities of nanoporous carbon calculated by density functional and M□ller-Plesset methods. *Physical Review B*, **2008**, 78,	3.3	46
345	Influence of nonlocal exchange-correlation effects on the response properties of simple metal clusters. *Physical Review B*, **1992**, 46, 4891-4898	3.3	46
344	Density-functional calculation of the fragmentation of doubly ionized spherical jelliumlike metallic microparticles. *Physical Review B*, **1986**, 34, 2152-2157	3.3	46
343	Theoretical study of icosahedral Ni clusters within the embedded-atom method. *Physical Review B*, **1996**, 54, 5961-5969	3.3	45
342	Prediction of the glass formation range of transition metal alloys. *Journal of Physics F: Metal Physics* , **1988**, 18, 2149-2157		45

341	Electronegativity scale for metals. *Physical Review B*, **1979**, 19, 3889-3895	3.3	45
340	Patching and tearing single-wall carbon-nanotube ropes into multiwall carbon nanotubes. *Physical Review Letters*, **2002**, 89, 255501	7.4	44
339	Embedded-atom method applied to bimetallic clusters: The Cu-Ni and Cu-Pd systems. *Physical Review B*, **1994**, 49, 16649-16658	3.3	44
338	Glass-forming ability in binary alloys produced by ion beam mixing and by laser quenching. *Materials Letters*, **1986**, 4, 316-319	3.3	43
337	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
336	Clusters and layers of C60 molecules supported on a graphite substrate. *Physical Review B*, **1997**, 55, 7190-7197	3.3	42
335	Half-metallic finite zigzag single-walled carbon nanotubes from first principles. *Physical Review B*, **2008**, 78,	3.3	42
334	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
333	A theoretical study of the static structure and thermodynamics of liquid lithium. *Journal of Physics Condensed Matter*, **1993**, 5, 4283-4298	1.8	41
332	An Application of Non-Extensive Statistical Mechanics to Nanosystems. *Journal of Computational and Theoretical Nanoscience*, **2004**, 1, 227-229	0.3	40
331	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
330	Coulomb barriers in the dissociation of doubly charged clusters. *Physical Review B*, **1991**, 43, 9459-9466	3.3	39
329	Charge transfer and heat of formation in CsCl intermetallic compounds. *Journal of Physics and Chemistry of Solids*, **1978**, 39, 79-87	3.9	39
328	Nonlocality and the energy of alloy formation. *Journal of Physics F: Metal Physics*, **1978**, 8, 2455-2460		39
327	Competition between molecular and dissociative adsorption of hydrogen on palladium clusters deposited on defective graphene. *RSC Advances*, **2015**, 5, 47945-47953	3.7	37
326	Structural and thermal properties of silicon-doped fullerenes. *Journal of Chemical Physics*, **2003**, 119, 1127-1135	3.9	37
325	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
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323	Adsorption of Lithium on Finite Graphitic Clusters. *Journal of Physical Chemistry C*, **2009**, 113, 939-941	3.8	34
322	Structural and thermal stability of narrow and short carbon nanotubes and nanostrips. *Carbon*, **2005**, 43, 1371-1377	10.4	34
321	Tight binding molecular dynamics studies of boron assisted nanotube growth. *Journal of Chemical Physics*, **2000**, 113, 3814-3821	3.9	34
320	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
319	Comparative ab initio studies of small tin and lead clusters. *Annalen Der Physik*, **1998**, 7, 107-119	2.6	34
318	Theoretical study of the photoabsorption spectrum of Na8, Na20, Cs8, and Cs10O clusters. *Physical Review B*, **1992**, 45, 13657-13663	3.3	34
317	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
316	Simulated porosity and electronic structure of nanoporous carbons. *Journal of Chemical Physics*, **2011**, 135, 104706	3.9	33
315	On the Factors Controlling Glass Forming Ability of Metallic Alloys Formed by Fast Liquid Quenching. *Physica Status Solidi A*, **1984**, 81, 55-61		33
314	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
313	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
312	Simulating the thermal behavior and fragmentation mechanisms of exohedral and substitutional silicon-doped C60. *Journal of Chemical Physics*, **2005**, 123, 204323	3.9	31
311	Calculation of metastable free-energy diagrams and glass formation in the Mg Cu Y alloy and its boundary binaries using the Miedema model. *Intermetallics*, **2006**, 14, 297-307	3.5	31
310	Adsorption and growth of palladium clusters on graphdiyne. *Physical Chemistry Chemical Physics*, **2017**, 19, 19094-19102	3.6	30
309	Magic numbers of sodium clusters. *Solid State Communications*, **1986**, 57, 85-88	1.6	30
308	Simulation of hydrogen storage in porous carbons. *Journal of Materials Research*, **2013**, 28, 589-604	2.5	28
307	Surface plasmon excitations in C60, C60K and C60H clusters. *Physica B: Condensed Matter*, **1993**, 183, 247-263	2.8	28
306	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

305	Thermal road for fullerene annealing. *Chemical Physics Letters*, **1997**, 273, 367-370	2.5	27
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297	Simulating the thermal stability and phase changes of small carbon clusters and fullerenes. *European Physical Journal D*, **1999**, 6, 221-233	1.3	24
296	Theoretical Models for the Optical Properties of Clusters and Nanostructures. *International Journal of Modern Physics B*, **1997**, 11, 2727-2776	1.1	23
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294	Controlling the Adsorption of Carbon Monoxide on Platinum Clusters by Dopant-Induced Electronic Structure Modification. *Angewandte Chemie*, **2016**, 128, 11225-11229	3.6	22
293	Theoretical study of molecular hydrogen clusters. *European Physical Journal D*, **2007**, 43, 61-64	1.3	22
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290	Conditions for the self-assembling of cluster materials. *Nanotechnology*, **2002**, 13, 253-257	3.4	22
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288	Dissociation channels of NaN+ clusters (3 . *Physical Review B*, **1990**, 41, 5595-5601	3.3	22

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278	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
277	First-Principles Structural and Electronic Characterization of Ordered SiO2 Nanowires. *Journal of Physical Chemistry C*, **2012**, 116, 18973-18982	3.8	20
276	Structure and energetics of Nan-xLix (n . *Physical Review B*, **1990**, 41, 5636-5642	3.3	20
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274	Theoretical study of the binding of Na clusters encapsulated in the C240 fullerene. *Physical Review B*, **1996**, 53, 16059-16066	3.3	19
273	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
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266	Immersion of hydrogen atoms in aluminium clusters. *Zeitschrift F□ Physik D-Atoms Molecules and Clusters*, **1989**, 13, 269-275		18
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264	Nonmetal-metal transition in Ni clusters. *Solid State Communications*, **1997**, 104, 635-639	1.6	17
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262	Dissociation of doubly charged alkali metal clusters. *Annalen Der Physik*, **1992**, 504, 270-280	2.6	17
261	Electronegativity of positive ions in the density functional theory. *Zeitschrift F□ Physik A*, **1982**, 305, 31-37		17
260	Optical Properties of Nanostructures from Time-Dependent Density Functional Theory. *Journal of Computational and Theoretical Nanoscience*, **2004**, 1, 231-255	0.3	17
259	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
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256	Electron density in simple metals. Relation to bulk and surface properties. *Journal of Physics F: Metal Physics*, **1980**, 10, 1995-2008		16
255	Theoretical study of the adsorption of hydrogen on cobalt clusters. *Physical Chemistry Chemical Physics*, **2018**, 20, 21163-21176	3.6	15
254	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
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252	Fragmentation and Coulomb explosion of deuterium clusters by the interaction with intense laser pulses. *Physical Review A*, **2005**, 72,	2.6	15

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249	Electronic structure of negatively charged aluminium clusters. *Physica B: Condensed Matter*, **1991**, 168, 32-38	2.8	15
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223	Coulomb explosion of charged jellium clusters. *Zeitschrift F□ Physik D-Atoms Molecules and Clusters* , **1989**, 11, 323-326		13
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