MarÃ-a J LÃ³pez

List of Publications by Year
in descending order

108 papers	3,697 citations	125106 35 h-index	150775 59 g-index
109 all docs	109 docs citations	109 times ranked	4184 citing authors

#	Article	IF	Citations
1	Palladium clusters, free and supported on surfaces, and their applications in hydrogen storage. Physical Chemistry Chemical Physics, 2022, 24, 2729-2751.	1.3	9
2	Catalytic activity of Coâ€“Ag nanoalloys to dissociate molecular hydrogen. New insights on the chemical environment. International Journal of Hydrogen Energy, 2022, 47, 19038-19050.	3.8	3
3	Infrared spectra and structures of C60Rhn+ complexes. Carbon, 2022, 197, 535-543.	5.4	7
4	Interaction of hydrogen with palladiumâ€“copper nanoalloys. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	7
5	Theoretical Study of the Diels-Alder Dimerization of C30H10. ECS Meeting Abstracts, 2021, MA2021-01, 645-645.	0.0	0
6	Adsorption of transition metal clusters on Boron-graphdiyne. Applied Surface Science, 2021, 548, 149270.	3.1	4
7	C60Con complexes as hydrogen adsorbing materials. International Journal of Hydrogen Energy, 2021, 46, 20594-20606.	3.8	7
8	Absence of spillover of hydrogen adsorbed on small palladium clusters anchored to graphene vacancies. Applied Surface Science, 2021, 559, 149835.	3.1	17
9	Nanoalloys of Metals Which Do Not Form Bulk Alloys: The Case of Agâ€“Co. Journal of Physical Chemistry A, 2020, 124, 6468-6477.	1.1	12
10	Dimerization of pentacyclopentacorannulene C30H10 as a strategy to produce C60H20 as a precursor for C60. RSC Advances, 2020, 10, 3689-3693.	1.7	3
11	Reactivity of Cobaltâ€Fullerene Complexes towards Deuterium. ChemPhysChem, 2020, 21, 1012-1018.	1.0	8
12	Interaction of Hydrogen with Graphitic Surfaces, Clean and Doped with Metal Clusters. , 2020, , 545-566.		0
13	Transferability in interatomic potentials for carbon. Carbon, 2019, 155, 624-634.	5.4	55
14	Dynamics of Cluster Isomerization Induced by Hydrogen Adsorption. Journal of Physical Chemistry C, 2019, 123, 15236-15243.	1.5	12
15	Bimetallic Alâ€“Sn clusters: mixing at the nanoscale. Physical Chemistry Chemical Physics, 2019, 21, 22919-22929.	1.3	8
16	Theoretical study of the adsorption of hydrogen on cobalt clusters. Physical Chemistry Chemical Physics, 2018, 20, 21163-21176.	1.3	19
17	Interaction of Hydrogen with Graphitic Surfaces, Clean and Doped with Metal Clusters. , 2018, , 1-22.		0
18	Competition between Palladium Clusters and Hydrogen to Saturate Graphene Vacancies. Journal of Physical Chemistry C, 2017, 121, 10843-10850.	1.5	21

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19	Structural prediction of graphitization and porosity in carbide-derived carbons. Carbon, 2017, 119, 1-9.	5.4	62
20	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.	1.1	25
21	Interaction of aromatic molecules with small gold clusters. Chemical Physics Letters, 2017, 684, 91-96.	1.2	10
22	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.	1.2	30
23	Manipulating the Magnetic Moment of Palladium Clusters by Adsorption and Dissociation of Molecular Hydrogen. Journal of Physical Chemistry C, 2017, 121, 20756-20762.	1.5	12
24	Adsorption and growth of palladium clusters on graphdiyne. Physical Chemistry Chemical Physics, 2017, 19, 19094-19102.	1.3	40
25	The Storage of Hydrogen in Nanoporous Carbons. Journal of the Mexican Chemical Society, 2017, 56, .	0.2	2
26	Is Spillover Relevant for Hydrogen Adsorption and Storage in Porous Carbons Doped with Palladium Nanoparticles?. Journal of Physical Chemistry C, 2016, 120, 17357-17364.	1.5	51
27	Interaction of hydrogen with palladium clusters deposited on graphene. AIP Conference Proceedings, 2015, , .	0.3	0
28	Competition between molecular and dissociative adsorption of hydrogen on palladium clusters deposited on defective graphene. RSC Advances, 2015, 5, 47945-47953.	1.7	45
29	From graphene oxide to pristine graphene: revealing the inner workings of the full structural restoration. Nanoscale, 2015, 7, 2374-2390.	2.8	95
30	Ab initio studies of propene epoxidation on oxidized silver surfaces. Physical Chemistry Chemical Physics, 2014, 16, 26546-26552.	1.3	17
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.	1.5	73
32	Simulation of hydrogen storage in porous carbons. Journal of Materials Research, 2013, 28, 589-604.	1.2	31
33	Evolution of the atomic structure and the magnetism of small oxygen clusters. Computational and Theoretical Chemistry, 2013, 1021, 215-221.	1.1	3
34	Electronic and magnetic properties of Fe clusters inside finite zigzag single-wall carbon nanotubes. Physical Review B, 2013, 87, .	1.1	8
35	Adsorption and dissociation of molecular hydrogen on the edges of graphene nanoribbons. Journal of Nanoparticle Research, 2012, 14, 1.	0.8	15
36	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.	0.6	0

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37	Adsorption and Dissociation of Molecular Hydrogen on Palladium Clusters Supported on Graphene. Journal of Physical Chemistry C, 2012, 116, 21179-21189.	1.5	104
38	Simulated porosity and electronic structure of nanoporous carbons. Journal of Chemical Physics, 2011, 135, 104706.	1.2	37
39	Simulation of the hydrogen storage in nanoporous carbons with different pore shapes. International Journal of Hydrogen Energy, 2011, 36, 10748-10759.	3.8	65
40	Modeling of the functionalization of single-wall carbon nanotubes towards its solubilization in an aqueous medium. European Physical Journal D, 2011, 61, 381-388.	0.6	14
41	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.	1.2	40
42	Theoretical study of the transition from planar to three-dimensional structures of palladium clusters supported on graphene. Physical Review B, 2010, 81, .	1.1	122
43	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.	7.2	246
44	Adsorption of Lithium on Finite Graphitic Clusters. Journal of Physical Chemistry C, 2009, 113, 939-941.	1.5	34
45	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.	1.5	12
46	Half-metallic finite zigzag single-walled carbon nanotubes from first principles. Physical Review B, 2008, 78, .	1.1	42
47	Hydrogen storage capacities of nanoporous carbon calculated by density functional and MÃ¸ller-Plesset methods. Physical Review B, 2008, 78, .	1.1	49
48	Interaction of narrow carbon nanotubes with nitronium tetrafluoroborate salts. Journal of Chemical Physics, 2008, 128, 214703.	1.2	6
49	Shape of the hydrogen adsorption regions of MOF-5 and its impact on the hydrogen storage capacity. Physical Review B, 2008, 78, .	1.1	13
50	Hydrogen storage in pure and Li-doped carbon nanopores: Combined effects of concavity and doping. Journal of Chemical Physics, 2008, 128, 144704.	1.2	53
51	Stability of silicon-doped C60 dimers. Journal of Chemical Physics, 2007, 126, 044705.	1.2	13
52	The optimum average nanopore size for hydrogen storage in carbon nanoporous materials. Carbon, 2007, 45, 2649-2658.	5.4	168
53	Density functional calculations of hydrogen adsorption on boron nanotubes and boron sheets. Nanotechnology, 2006, 17, 778-785.	1.3	83
54	Density functional study of molecular hydrogen coverage on carbon nanotubes. Computational Materials Science, 2006, 35, 238-242.	1.4	54

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55	Buckling in boron sheets and nanotubes. Physica Status Solidi (A) Applications and Materials Science, 2006, 203, 1105-1110.	0.8	22
56	Electrostrictive deformations in small carbon clusters, hydrocarbon molecules, and carbon nanotubes. Physical Review A, 2006, 74, .	1.0	5
57	Structural and thermal stability of narrow and short carbon nanotubes and nanostrips. Carbon, 2005, 43, 1371-1377.	5.4	38
58	Adsorption of hydrogen on normal and pentaheptite single wall carbon nanotubes. European Physical Journal D, 2005, 34, 279-282.	0.6	25
59	BeB2nanostructures: A density functional study. Physical Review B, 2005, 72, .	1.1	6
60	Simulating the thermal behavior and fragmentation mechanisms of exohedral and substitutional silicon-doped C60. Journal of Chemical Physics, 2005, 123, 204323.	1.2	33
61	Theoretical study of the reactivity of cesium with benzene and graphitic CxHy clusters. Journal of Chemical Physics, 2005, 123, 074303.	1.2	7
62	Enhancement of hydrogen physisorption on graphene and carbon nanotubes by Li doping. Journal of Chemical Physics, 2005, 123, 204721.	1.2	247
63	Interaction of Molecular and Atomic Hydrogen With Single-Wall Carbon Nanotubes. IEEE Nanotechnology Magazine, 2004, 3, 304-310.	1.1	33
64	Growth Ability and Stability Indices of Clusters. Journal of Cluster Science, 2003, 14, 31-47.	1.7	7
65	Tight binding studies of exohedral silicon doped C60. Composites Science and Technology, 2003, 63, 1499-1505.	3.8	8
66	Structural and thermal properties of silicon-doped fullerenes. Journal of Chemical Physics, 2003, 119, 1127-1135.	1.2	39
67	Ab initiomolecular dynamics simulations of the two-step melting of NaSn. Physical Review B, 2003, 68, .	1.1	1
68	Analysis of the bonding and reactivity of H and the Al13 cluster using density functional concepts. Journal of Chemical Physics, 2003, 119, 5128-5141.	1.2	55
69	Interaction of molecular and atomic hydrogen with single-wall carbon nanotubes. , 2003, , .		1
70	Deformations and thermal stability of carbon nanotube ropes. , 2003, , .		1
71	Patching and Tearing Single-Wall Carbon-Nanotube Ropes into Multiwall Carbon Nanotubes. Physical Review Letters, 2002, 89, 255501.	2.9	52
72	Conditions for the self-assembling of cluster materials. Nanotechnology, 2002, 13, 253-257.	1.3	23

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73	Some Properties of a Model Liquid of C 60 Buckyballs. Physics and Chemistry of Liquids, 2002, 40, 457-467.	0.4	3
74	Interaction of molecular and atomic hydrogen with (5,5) and (6,6) single-wall carbon nanotubes. Journal of Chemical Physics, 2002, 117, 2281-2288.	1.2	198
75	Computer simulation of cluster assembling. International Journal of Quantum Chemistry, 2002, 86, 226-238.	1.0	18
76	ELECTRONIC SHELL EFFECTS IN METAL CLUSTERS AND THEIR CONSEQUENCES FOR CLUSTER SELF-ASSEMBLING. , 2002, , 1476-1507.		2
77	Assembling of hydrogenated aluminum clusters. European Physical Journal D, 2001, 16, 285-288.	0.6	16
78	Novel Polygonized Single-Wall Carbon Nanotube Bundles. Physical Review Letters, 2001, 86, 3056-3059.	2.9	113
79	Computer simulation of the spreading of metallic clusters landing at grazing incidence on a metallic surface. Physical Review B, 2000, 62, 16031-16039.	1.1	10
80	Interaction of lithium atoms with graphitic walls. AIP Conference Proceedings, 2000, , .	0.3	0
81	Molecular dynamics study of cluster impact on the (001) and (110) surfaces of fcc metals. Computational Materials Science, 2000, 17, 515-519.	1.4	10
82	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.	1.1	59
83	On the problem of fitting many-body potentials. I. The minimal maximum error scheme and the paradigm of metal systems. Journal of Chemical Physics, 1999, 110, 8899-8911.	1.2	43
84	Simulating the thermal stability and phase changes of small carbon clusters and fullerenes. European Physical Journal D, 1999, 6, 221-233.	0.6	25
85	Electronic Structure of Bimetallic Clusters Based on Alkali Elements. Springer Series in Cluster Physics, 1999, , 255-276.	0.3	0
86	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.	1.2	17
87	Mixed lead-alkali clusters in the gas phase and in liquid alloys. International Journal of Quantum Chemistry, 1998, 69, 341-348.	1.0	5
88	Magnetic moments of Ni clusters. Physical Review B, 1998, 57, 12469-12475.	1.1	73
89	Comparative ab initio studies of small tin and lead clusters. Annalen Der Physik, 1998, 7, 107-119.	0.9	35
90	Theoretical Study of the Collective Electronic Excitations of the Endohedral Clusters Na N @C780. , 1998, , 133-141.		0

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91	Geometrical effects on the magnetism of small Ni clusters. Physical Review B, 1997, 55, 13279-13282.	1.1	48
92	Thermal behaviour of carbon clusters and small fullerenes. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1997, 40, 385-388.	1.0	6
93	Study of clusters of interest for liquid ionic alloys. Annalen Der Physik, 1997, 509, 35-44.	0.9	6
94	Ionic vibrational breathing mode of metallic clusters. International Journal of Quantum Chemistry, 1997, 61, 613-626.	1.0	6
95	Thermal road for fullerene annealing. Chemical Physics Letters, 1997, 273, 367-370.	1.2	29
96	Theoretical study of icosahedral Ni clusters within the embedded-atom method. Physical Review B, 1996, 54, 5961-5969.	1.1	49
97	Structural and dynamical properties of Cuâ€“Au bimetallic clusters. Journal of Chemical Physics, 1996, 104, 1056-1066.	1.2	122
98	Theoretical study of the binding of Na clusters encapsulated in theC240fullerene. Physical Review B, 1996, 53, 16059-16066.	1.1	22
99	Vibrational frequencies of sodium clusters. International Journal of Quantum Chemistry, 1995, 56, 589-601.	1.0	7
100	Fragmentation of atomic clusters: A theoretical study. Physical Review A, 1994, 50, 1445-1458.	1.0	76
101	Pion-nucleus elastic scattering in a local approximation to the delta-hole model. Nuclear Physics A, 1991, 526, 685-702.	0.6	66
102	Stability of isomeric Na n clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1991, 19, 141-143.	1.0	7
103	Evaporation rates of hot sodium clusters. , 1991, , 569-572.		0
104	Atomic structure and segregation in alkali-metal heteroclusters. Physical Review B, 1990, 42, 5000-5008.	1.1	26
105	Dissociation channels ofNaN+clusters (3â‰¤Nâ‰¤37). Physical Review B, 1990, 41, 5595-5601.	1.1	22
106	Structure and energetics ofNanâ^'xLix(nâ‰¤21) clusters. Physical Review B, 1990, 41, 5636-5642.	1.1	21
107	Pionic distorsion factors for radiative pion capture studies. Physics Letters, Section B: Nuclear, Elementary Particle and High-Energy Physics, 1989, 222, 329-332.	1.5	3
108	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