Luis M Molina

List of Publications by Year
in descending order

44 papers	4,351 citations	257450 24 h-index	276875 41 g-index
46 all docs	46 docs citations	46 times ranked	4650 citing authors

#	Article	IF	Citations
1	Oxygen vacancies on TiO2(110) and their interaction with H2O and O2: A combined high-resolution STM and DFT study. Surface Science, 2005, 598, 226-245.	1.9	560
2	Active Role of Oxide Support during CO Oxidation atAu/MgO. Physical Review Letters, 2003, 90, 206102.	7.8	431
3	Adsorption of O2 and oxidation of CO at Au nanoparticles supported by TiO2(110). Journal of Chemical Physics, 2004, 120, 7673-7680.	3.0	294
4	Guanine Quartet Networks Stabilized by Cooperative Hydrogen Bonds. Angewandte Chemie - International Edition, 2005, 44, 2270-2275.	13.8	275
5	Density functional study of adsorption of molecular hydrogen on graphene layers. Journal of Chemical Physics, 2000, 112, 8114-8119.	3.0	261
6	Adsorption, diffusion, and dissociation of molecular oxygen at defected TiO2(110): A density functional theory study. Journal of Chemical Physics, 2004, 120, 988-997.	3.0	251
7	Theoretical study of CO oxidation on Au nanoparticles supported by MgO(100). Physical Review B, 2004, 69, .	3.2	246
8	Selective Propene Epoxidation on Immobilized Au_{6â€“10} Clusters: The Effect of Hydrogen and Water on Activity and Selectivity. Angewandte Chemie - International Edition, 2009, 48, 1467-1471.	13.8	246
9	Some recent theoretical advances in the understanding of the catalytic activity of Au. Applied Catalysis A: General, 2005, 291, 21-31.	4.3	240
10	Interaction of molecular and atomic hydrogen with (5,5) and (6,6) single-wall carbon nanotubes. Journal of Chemical Physics, 2002, 117, 2281-2288.	3.0	198
11	Interaction of lithium with graphene: Anab initiostudy. Physical Review B, 2004, 70, .	3.2	171
12	Theoretical study of thiol-induced reconstructions on the Au(111) surface. Chemical Physics Letters, 2002, 360, 264-271.	2.6	161
13	The activity of the tetrahedral Au20 cluster: charging and impurity effects. Journal of Catalysis, 2005, 233, 399-404.	6.2	124
14	Size-dependent selectivity and activity of silver nanoclusters in the partial oxidation of propylene to propylene oxide and acrolein: A joint experimental and theoretical study. Catalysis Today, 2011, 160, 116-130.	4.4	115
15	Growth of Unidirectional Molecular Rows of Cysteine onAu(110)â”(1Ã—2)Driven by Adsorbate-Induced Surface Rearrangements. Physical Review Letters, 2004, 93, 086101.	7.8	112
16	Oxygen adsorption at anionic free and supported Au clusters. Journal of Chemical Physics, 2005, 123, 161104.	3.0	76
17	Chemical Properties of Small Au Clusters:â€‰ An Analysis of the Local Site Reactivity. Journal of Physical Chemistry C, 2007, 111, 6668-6677.	3.1	72
18	Guanine Quartet Networks Stabilized by Cooperative Hydrogen Bonds. Angewandte Chemie, 2005, 117, 2310-2315.	2.0	64

#	Article	IF	Citations
19	Promoting and poisoning effects of Na and Cl coadsorption on CO oxidation over MgO-supported Au nanoparticles. Journal of Catalysis, 2004, 227, 217-226.	6.2	61
20	Controlling the Adsorption of Carbon Monoxide on Platinum Clusters by Dopantâ€Induced Electronic Structure Modification. Angewandte Chemie - International Edition, 2016, 55, 11059-11063.	13.8	55
21	Structural and thermal properties of silicon-doped fullerenes. Journal of Chemical Physics, 2003, 119, 1127-1135.	3.0	39
22	Interaction of Molecular and Atomic Hydrogen With Single-Wall Carbon Nanotubes. IEEE Nanotechnology Magazine, 2004, 3, 304-310.	2.0	33
23	Melting behavior of large disordered sodium clusters. European Physical Journal D, 2001, 15, 221-227.	1.3	29
24	Water adsorption and dissociation on gold catalysts supported on anatase-TiO2(101). Applied Surface Science, 2019, 487, 244-252.	6.1	27
25	Controlling the Adsorption of Carbon Monoxide on Platinum Clusters by Dopantâ€Induced Electronic Structure Modification. Angewandte Chemie, 2016, 128, 11225-11229.	2.0	25
26	Conditions for the self-assembling of cluster materials. Nanotechnology, 2002, 13, 253-257.	2.6	23
27	Structural models of inorganic fullerene-like structures. Surface Science, 2003, 526, 243-247.	1.9	19
28	Computer simulation of cluster assembling. International Journal of Quantum Chemistry, 2002, 86, 226-238.	2.0	18
29	New insights on the reaction mechanisms for CO oxidation on Au catalysts. Chemical Physics Letters, 2009, 468, 201-204.	2.6	18
30	Ab initio calculations for mixed clusters of lead and alkali elements, and implications for the structure of their solid and liquid alloys. Chemical Physics Letters, 1998, 289, 451-456.	2.6	17
31	Ab initio studies of propene epoxidation on oxidized silver surfaces. Physical Chemistry Chemical Physics, 2014, 16, 26546-26552.	2.8	17
32	Assembling of hydrogenated aluminum clusters. European Physical Journal D, 2001, 16, 285-288.	1.3	16
33	Ab initio studies of ethanol dehydrogenation at binary AuPd nanocatalysts. Molecular Catalysis, 2018, 449, 8-13.	2.0	14
34	Assembling alkaliâ€“lead solid compounds from clusters. Journal of Chemical Physics, 1999, 111, 7053-7061.	3.0	10
35	Interaction of aromatic molecules with small gold clusters. Chemical Physics Letters, 2017, 684, 91-96.	2.6	10
36	Building alkali-lead intermetallic compounds from clusters. Solid State Communications, 1998, 108, 519-524.	1.9	8

#	Article	IF	Citations
37	BeB2nanostructures: A density functional study. Physical Review B, 2005, 72, .	3.2	6
38	Mixed lead-alkali clusters in the gas phase and in liquid alloys. International Journal of Quantum Chemistry, 1998, 69, 341-348.	2.0	5
39	Octet composition in alkali-Pb solid alloys. Physical Review B, 2002, 66, .	3.2	1
40	Ab initiomolecular dynamics simulations of the two-step melting of NaSn. Physical Review B, 2003, 68, .	3.2	1
41	Interaction of molecular and atomic hydrogen with single-wall carbon nanotubes. , 2003, , .		1
42	Hydrogen and Hydrogen Clusters Across Disciplines. Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems, 2010, , 299-342.	0.6	0
43	Ab initio studies of propene oxide formation at gold nanocatalysts supported on anatase-TiO2. Molecular Catalysis, 2020, 486, 110855.	2.0	0
44	Theoretical Description and Modeling of Hydrogen Bonds at Solid Surfaces. , 2018, , 175-180.		0