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	Ab initio studies of propene oxide formation at gold nanocatalysts supported on anatase-TiO2. Molecular Catalysis, 2020, 486, 110855.	2.0	0
2	Water adsorption and dissociation on gold catalysts supported on anatase-TiO2(101). Applied Surface Science, 2019, 487, 244-252.	6.1	27
3	Ab initio studies of ethanol dehydrogenation at binary AuPd nanocatalysts. Molecular Catalysis, 2018, 449, 8-13.	2.0	14
4	Theoretical Description and Modeling of Hydrogen Bonds at Solid Surfaces. , 2018, , 175-180.		0
5	Interaction of aromatic molecules with small gold clusters. Chemical Physics Letters, 2017, 684, 91-96.	2.6	10
6	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
7	Controlling the Adsorption of Carbon Monoxide on Platinum Clusters by Dopantâ€Induced Electronic Structure Modification. Angewandte Chemie, 2016, 128, 11225-11229.	2.0	25
8	Ab initio studies of propene epoxidation on oxidized silver surfaces. Physical Chemistry Chemical Physics, 2014, 16, 26546-26552.	2.8	17
9	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
10	Hydrogen and Hydrogen Clusters Across Disciplines. Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems, 2010, , 299-342.	0.6	0
11	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
12	New insights on the reaction mechanisms for CO oxidation on Au catalysts. Chemical Physics Letters, 2009, 468, 201-204.	2.6	18
13	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
14	The activity of the tetrahedral Au20 cluster: charging and impurity effects. Journal of Catalysis, 2005, 233, 399-404.	6.2	124
15	Guanine Quartet Networks Stabilized by Cooperative Hydrogen Bonds. Angewandte Chemie - International Edition, 2005, 44, 2270-2275.	13.8	275
16	Guanine Quartet Networks Stabilized by Cooperative Hydrogen Bonds. Angewandte Chemie, 2005, 117, 2310-2315.	2.0	64
17	Some recent theoretical advances in the understanding of the catalytic activity of Au. Applied Catalysis A: General, 2005, 291, 21-31.	4.3	240
18	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

#	Article	IF	Citations
19	Oxygen adsorption at anionic free and supported Au clusters. Journal of Chemical Physics, 2005, 123, 161104.	3.0	76
20	BeB2nanostructures: A density functional study. Physical Review B, 2005, 72, .	3.2	6
21	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
22	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
23	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
24	Interaction of Molecular and Atomic Hydrogen With Single-Wall Carbon Nanotubes. IEEE Nanotechnology Magazine, 2004, 3, 304-310.	2.0	33
25	Interaction of lithium with graphene: Anab initiostudy. Physical Review B, 2004, 70, .	3.2	171
26	Theoretical study of CO oxidation on Au nanoparticles supported by MgO(100). Physical Review B, 2004, 69, .	3.2	246
27	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
28	Structural models of inorganic fullerene-like structures. Surface Science, 2003, 526, 243-247.	1.9	19
29	Active Role of Oxide Support during CO Oxidation atAu/MgO. Physical Review Letters, 2003, 90, 206102.	7.8	431
30	Structural and thermal properties of silicon-doped fullerenes. Journal of Chemical Physics, 2003, 119, 1127-1135.	3.0	39
31	Ab initiomolecular dynamics simulations of the two-step melting of NaSn. Physical Review B, 2003, 68, .	3.2	1
32	Interaction of molecular and atomic hydrogen with single-wall carbon nanotubes. , 2003, , .		1
33	Conditions for the self-assembling of cluster materials. Nanotechnology, 2002, 13, 253-257.	2.6	23
34	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
35	Octet composition in alkali-Pb solid alloys. Physical Review B, 2002, 66, .	3.2	1
36	Computer simulation of cluster assembling. International Journal of Quantum Chemistry, 2002, 86, 226-238.	2.0	18

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37	Theoretical study of thiol-induced reconstructions on the Au(111) surface. Chemical Physics Letters, 2002, 360, 264-271.	2.6	161
38	Melting behavior of large disordered sodium clusters. European Physical Journal D, 2001, 15, 221-227.	1.3	29
39	Assembling of hydrogenated aluminum clusters. European Physical Journal D, 2001, 16, 285-288.	1.3	16
40	Density functional study of adsorption of molecular hydrogen on graphene layers. Journal of Chemical Physics, 2000, 112, 8114-8119.	3.0	261
41	Assembling alkaliâ€“lead solid compounds from clusters. Journal of Chemical Physics, 1999, 111, 7053-7061.	3.0	10
42	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
43	Mixed lead-alkali clusters in the gas phase and in liquid alloys. International Journal of Quantum Chemistry, 1998, 69, 341-348.	2.0	5
44	Building alkali-lead intermetallic compounds from clusters. Solid State Communications, 1998, 108, 519-524.	1.9	8