Olga Lopez-Acevedo

List of Publications by Citations

48 papers	4,622 citations	23 h-index	50 g-index
50 ext. papers	5,085 ext. citations	5.2 avg, IF	5.1 L-index

#	Paper	IF	Citations
48	A unified view of ligand-protected gold clusters as superatom complexes. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 9157-62	11.5	1264
47	Electronic structure calculations with GPAW: a real-space implementation of the projector augmented-wave method. *Journal of Physics Condensed Matter*, **2010**, 22, 253202	1.8	1092
46	Chirality and electronic structure of the thiolate-protected Au38 nanocluster. *Journal of the American Chemical Society*, **2010**, 132, 8210-8	16.4	367
45	Structure and Bonding in the Ubiquitous Icosahedral Metallic Gold Cluster Au144(SR)60. *Journal of Physical Chemistry C*, **2009**, 113, 5035-5038	3.8	363
44	Quantum size effects in ambient CO oxidation catalysed by ligand-protected gold clusters. *Nature Chemistry*, **2010**, 2, 329-34	17.6	266
43	Piezoelectric coefficients and spontaneous polarization of ScAlN. *Journal of Physics Condensed Matter*, **2015**, 27, 245901	1.8	119
42	Silver (I) as DNA glue: Ag(+)-mediated guanine pairing revealed by removing Watson-Crick constraints. *Scientific Reports*, **2015**, 5, 10163	4.9	101
41	Thiolate-Protected Au25 Superatoms as Building Blocks: Dimers and Crystals *Journal of Physical Chemistry C*, **2010**, 114, 15986-15994	3.8	99
40	A density functional investigation of thiolate-protected bimetal PdAu(24)(SR)(18)(z) clusters: doping the superatom complex. *Physical Chemistry Chemical Physics*, **2009**, 11, 7123-9	3.6	92
39	Electronic and vibrational signatures of the Au102(p-MBA)44 cluster. *Journal of the American Chemical Society*, **2011**, 133, 3752-5	16.4	74
38	Density functional theory based screening of ternary alkali-transition metal borohydrides: a computational material design project. *Journal of Chemical Physics*, **2009**, 131, 014101	3.9	74
37	Experimental and Density Functional Theory Analysis of Serial Introductions of Electron-Withdrawing Ligands into the Ligand Shell of a Thiolate-Protected Au25 Nanoparticle. *Journal of Physical Chemistry C*, **2010**, 114, 8276-8281	3.8	59
36	Orbital-free density functional theory implementation with the projector augmented-wave method. *Journal of Chemical Physics*, **2014**, 141, 234102	3.9	58
35	Theoretical Characterization of Cyclic Thiolated Copper, Silver, and Gold Clusters. *Journal of Physical Chemistry C*, **2010**, 114, 13571-13576	3.8	46
34	Oligomeric Gold thiolate Units Define the Properties of the Molecular Junction between Gold and Benzene Dithiols. *Journal of Physical Chemistry Letters*, **2010**, 1, 1528-1532	6.4	40
33	Evidence of superatom electronic shells in ligand-stabilized aluminum clusters. *Journal of Chemical Physics*, **2011**, 135, 094701	3.9	40
32	The Al50Cp*12 Cluster A 138-Electron Closed Shell (L = 6) Superatom. *European Journal of Inorganic Chemistry*, **2011**, 2011, 2649-2652	2.3	39

31	Atomic and electronic structure of tetrahedral amorphous carbon surfaces from density functional theory: Properties and simulation strategies. *Carbon*, **2014**, 77, 1168-1182	10.4	37
30	The Role of Hydrogen Bonds in the Stabilization of Silver-Mediated Cytosine Tetramers. *Journal of Physical Chemistry Letters*, **2015**, 6, 4061-6	6.4	37
29	Electronic structure of gold, aluminum, and gallium superatom complexes. *Physical Review B*, **2011**, 84,	3.3	37
28	Optical Spectra of the Special Au144 Gold-Cluster Compounds: Sensitivity to Structure and Symmetry. *Journal of Physical Chemistry C*, **2015**, 119, 11250-11259	3.8	34
27	Grid-Based Projector Augmented Wave (GPAW) Implementation of Quantum Mechanics/Molecular Mechanics (QM/MM) Electrostatic Embedding and Application to a Solvated Diplatinum Complex. *Journal of Chemical Theory and Computation*, **2017**, 13, 6010-6022	6.4	24
26	Accurate schemes for calculation of thermodynamic properties of liquid mixtures from molecular dynamics simulations. *Journal of Chemical Physics*, **2016**, 145, 244504	3.9	23
25	Silver-Mediated Double Helix: Structural Parameters for a Robust DNA Building Block. *ACS Omega*, **2017**, 2, 7343-7348	3.9	19
24	Quantum walks on Cayley graphs. *Journal of Physics A*, **2006**, 39, 585-599		18
23	Three-Dimensional Uracil Network with Sodium as a Linker. *Journal of Physical Chemistry C*, **2016**, 120, 26342-26349	3.8	17
22	Structural morphology of carbon nanofibers grown on different substrates. *Carbon*, **2016**, 98, 343-351	10.4	17
21	Characterization of iron-carbonyl-protected gold clusters. *Journal of the American Chemical Society*, **2009**, 131, 12573-5	16.4	17
20	On the interaction between gold and silver metal atoms and DNA/RNA nucleobases – a comprehensive computational study of ground state properties. *Nanotechnology Reviews*, **2015**, 4,	6.3	14
19	Solvent driven formation of silver embedded resorcinarene nanorods. *CrystEngComm*, **2012**, 14, 347-350	3.3	13
18	Redox Potentials from Ab Initio Molecular Dynamics and Explicit Entropy Calculations: Application to Transition Metals in Aqueous Solution. *Journal of Chemical Theory and Computation*, **2017**, 13, 3432-3441	6.4	12
17	Derivatives of the thiolate-protected gold cluster Au25(SR)18 -1. *European Physical Journal D*, **2011**, 63, 311-314	1.3	12
16	Optimizing a parametrized Thomas-Fermi-Dirac-Weizsäcker density functional for atoms. *Physical Chemistry Chemical Physics*, **2015**, 17, 31463-71	3.6	11
15	Excitation-dependent fluorescence from atomic/molecular layer deposited sodium-uracil thin films. *Scientific Reports*, **2017**, 7, 6982	4.9	11
14	Silver-Stabilized Guanine Duplex: Structural and Optical Properties. *Journal of Physical Chemistry Letters*, **2018**, 9, 4789-4794	6.4	9

13	Energy band alignment and electronic states of amorphous carbon surfaces in vacuo and in aqueous environment. *Journal of Applied Physics*, **2015**, 117, 034502	2.5	9
12	Semilocal kinetic energy functionals with parameters from neutral atoms. *Physical Review B*, **2019**, 100,	3.3	8
11	Atomic structure and origin of chirality of DNA-stabilized silver clusters. *Physical Review Materials*, **2020**, 4,	3.2	7
10	First-Principles Study of Excited State Evolution in a Protected Gold Complex. *Journal of Physical Chemistry C*, **2013**, 117, 11837-11842	3.8	6
9	Real-time time-dependent density functional theory implementation of electronic circular dichroism applied to nanoscale metal-organic clusters. *Journal of Chemical Physics*, **2021**, 154, 114102	3.9	6
8	Optical Properties of Silver-Mediated DNA from Molecular Dynamics and Time Dependent Density Functional Theory. *International Journal of Molecular Sciences*, **2018**, 19,	6.3	5
7	Self-consistent assessment of Englert-Schwinger model on atomic properties. *Journal of Chemical Physics*, **2017**, 147, 234102	3.9	4
6	Density and localized statesRimpact on amorphous carbon electron transport mechanisms. *Journal of Applied Physics*, **2016**, 120, 214303	2.5	2
5	Ab initio metadynamics determination of temperature-dependent free-energy landscape in ultrasmall silver clusters.. *Journal of Chemical Physics*, **2022**, 156, 154301	3.9	2
4	Conductance through atomic point contacts between fcc(100) electrodes of gold. *European Physical Journal B*, **2008**, 66, 497-501	1.2	1
3	Large-Z limit in atoms and solids from first principles. *Journal of Chemical Physics*, **2019**, 151, 244101	3.9	1
2	A Multiscale Code for Flexible Hybrid Simulations Using ASE Framework. *Computing in Science and Engineering*, **2014**, 16, 54-62	1.5	
1	Probing the Atomic-Scale Structure of Monolayer-Protected Au38 Clusters. *Microscopy and Microanalysis*, **2010**, 16, 1652-1653	0.5	