

# Olga Lopez-Acevedo

## List of Publications by Year in descending order

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48  
papers

5,578  
citations

279487

23  
h-index

197535

49  
g-index

50  
all docs

50  
docs citations

50  
times ranked

5904  
citing authors

#	ARTICLE	IF	CITATIONS
1	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, 9157-9162.	3.3	1,472
2	Electronic structure calculations with GPAW: a real-space implementation of the projector augmented-wave method. Journal of Physics Condensed Matter, 2010, 22, 253202.	0.7	1,451
3	Chirality and Electronic Structure of the Thiolate-Protected Au <sub>38</sub> Nanocluster. Journal of the American Chemical Society, 2010, 132, 8210-8218.	6.6	401
4	Structure and Bonding in the Ubiquitous Icosahedral Metallic Gold Cluster Au <sub>144</sub> (SR) <sub>60</sub> . Journal of Physical Chemistry C, 2009, 113, 5035-5038.	1.5	393
5	Quantum size effects in ambient CO oxidation catalysed by ligand-protected gold clusters. Nature Chemistry, 2010, 2, 329-334.	6.6	295
6	Piezoelectric coefficients and spontaneous polarization of ScAlN. Journal of Physics Condensed Matter, 2015, 27, 245901.	0.7	209
7	Silver (I) as DNA glue: Ag <sup>+</sup> -mediated guanine pairing revealed by removing Watson-Crick constraints. Scientific Reports, 2015, 5, 10163.	1.6	127
8	Thiolate-Protected Au <sub>25</sub> Superatoms as Building Blocks: Dimers and Crystals. Journal of Physical Chemistry C, 2010, 114, 15986-15994.	1.5	109
9	A density functional investigation of thiolate-protected bimetal PdAu <sub>24</sub> (SR) <sub>18</sub> z clusters: doping the superatom complex. Physical Chemistry Chemical Physics, 2009, 11, 7123.	1.3	100
10	Electronic and Vibrational Signatures of the Au <sub>102</sub> (P-MBA) <sub>44</sub> Cluster. Journal of the American Chemical Society, 2011, 133, 3752-3755.	6.6	80
11	Density functional theory based screening of ternary alkali-transition metal borohydrides: A computational material design project. Journal of Chemical Physics, 2009, 131, 014101.	1.2	77
12	Orbital-free density functional theory implementation with the projector augmented-wave method. Journal of Chemical Physics, 2014, 141, 234102.	1.2	74
13	Experimental and Density Functional Theory Analysis of Serial Introductions of Electron-Withdrawing Ligands into the Ligand Shell of a Thiolate-Protected Au <sub>25</sub> Nanoparticle. Journal of Physical Chemistry C, 2010, 114, 8276-8281.	1.5	61
14	Theoretical Characterization of Cyclic Thiolated Copper, Silver, and Gold Clusters. Journal of Physical Chemistry C, 2010, 114, 13571-13576.	1.5	51
15	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.	2.1	43
16	The Role of Hydrogen Bonds in the Stabilization of Silver-Mediated Cytosine Tetramers. Journal of Physical Chemistry Letters, 2015, 6, 4061-4066.	2.1	43
17	Evidence of superatom electronic shells in ligand-stabilized aluminum clusters. Journal of Chemical Physics, 2011, 135, 094701.	1.2	42
18	The Al <sub>50</sub> Cp* <sub>12</sub> Cluster - A 138-Electron Closed Shell (L = 6) Superatom. European Journal of Inorganic Chemistry, 2011, 2011, 2649-2652.	1.0	41

#	ARTICLE	IF	CITATIONS
19	Atomic and electronic structure of tetrahedral amorphous carbon surfaces from density functional theory: Properties and simulation strategies. <i>Carbon</i> , 2014, 77, 1168-1182.	5.4	41
20	Electronic structure of gold, aluminum, and gallium superatom complexes. <i>Physical Review B</i> , 2011, 84, .	1.1	39
21	Accurate schemes for calculation of thermodynamic properties of liquid mixtures from molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2016, 145, 244504.	1.2	38
22	Optical Spectra of the Special Au <sub>144</sub> Gold-Cluster Compounds: Sensitivity to Structure and Symmetry. <i>Journal of Physical Chemistry C</i> , 2015, 119, 11250-11259.	1.5	37
23	Grid-Based Projector Augmented Wave (GPAW) Implementation of Quantum Mechanics/Molecular Mechanics (QM/MM) Electrostatic Embedding and Application to a Solvated Diplatinum Complex. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 6010-6022.	2.3	32
24	Silver-Mediated Double Helix: Structural Parameters for a Robust DNA Building Block. <i>ACS Omega</i> , 2017, 2, 7343-7348.	1.6	26
25	Structural morphology of carbon nanofibers grown on different substrates. <i>Carbon</i> , 2016, 98, 343-351.	5.4	25
26	Quantum walks on Cayley graphs. <i>Journal of Physics A</i> , 2006, 39, 585-599.	1.6	23
27	On the interaction between gold and silver metal atoms and DNA/RNA nucleobases – a comprehensive computational study of ground state properties. <i>Nanotechnology Reviews</i> , 2015, 4, 173-191.	2.6	23
28	Three-Dimensional Uracil Network with Sodium as a Linker. <i>Journal of Physical Chemistry C</i> , 2016, 120, 26342-26349.	1.5	18
29	Redox Potentials from Ab Initio Molecular Dynamics and Explicit Entropy Calculations: Application to Transition Metals in Aqueous Solution. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3432-3441.	2.3	18
30	Characterization of Iron <sup>+</sup> Carbonyl-Protected Gold Clusters. <i>Journal of the American Chemical Society</i> , 2009, 131, 12573-12575.	6.6	17
31	Optimizing a parametrized Thomas-Fermi-Dirac-Weizsäcker density functional for atoms. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 31463-31471.	1.3	16
32	Real-time time-dependent density functional theory implementation of electronic circular dichroism applied to nanoscale metal-organic clusters. <i>Journal of Chemical Physics</i> , 2021, 154, 114102.	1.2	16
33	Silver-Stabilized Guanine Duplex: Structural and Optical Properties. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 4789-4794.	2.1	15
34	Derivatives of the thiolate-protected gold cluster Au <sub>25</sub> (SR) <sub>18</sub> -1. <i>European Physical Journal D</i> , 2011, 63, 311-314.	0.6	13
35	Solvent driven formation of silver embedded resorcinarene nanorods. <i>CrystEngComm</i> , 2012, 14, 347-350.	1.3	13
36	Excitation-dependent fluorescence from atomic/molecular layer deposited sodium-uracil thin films. <i>Scientific Reports</i> , 2017, 7, 6982.	1.6	13

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37	Atomic structure and origin of chirality of DNA-stabilized silver clusters. <i>Physical Review Materials</i> , 2020, 4, .	0.9	13
38	Semilocal kinetic energy functionals with parameters from neutral atoms. <i>Physical Review B</i> , 2019, 100, .	1.1	10
39	Energy band alignment and electronic states of amorphous carbon surfaces in vacuo and in aqueous environment. <i>Journal of Applied Physics</i> , 2015, 117, 034502.	1.1	9
40	Optical Properties of Silver-Mediated DNA from Molecular Dynamics and Time Dependent Density Functional Theory. <i>International Journal of Molecular Sciences</i> , 2018, 19, 2346.	1.8	7
41	First-Principles Study of Excited State Evolution in a Protected Gold Complex. <i>Journal of Physical Chemistry C</i> , 2013, 117, 11837-11842.	1.5	6
42	A Multiscale Code for Flexible Hybrid Simulations Using ASE Framework. <i>Computing in Science and Engineering</i> , 2014, 16, 54-62.	1.2	4
43	Self-consistent assessment of Englert-Schwinger model on atomic properties. <i>Journal of Chemical Physics</i> , 2017, 147, 234102.	1.2	4
44	<i>Ab initio</i> metadynamics determination of temperature-dependent free-energy landscape in ultrasmall silver clusters. <i>Journal of Chemical Physics</i> , 2022, 156, 154301.	1.2	4
45	Density and localized states' impact on amorphous carbon electron transport mechanisms. <i>Journal of Applied Physics</i> , 2016, 120, 214303.	1.1	3
46	Large-Z limit in atoms and solids from first principles. <i>Journal of Chemical Physics</i> , 2019, 151, 244101.	1.2	2
47	Conductance through atomic point contacts between fcc(100) electrodes of gold. <i>European Physical Journal B</i> , 2008, 66, 497-501.	0.6	1
48	Probing the Atomic-Scale Structure of Monolayer-Protected Au <sub>38</sub> Clusters. <i>Microscopy and Microanalysis</i> , 2010, 16, 1652-1653.	0.2	0