

Olga Lopez-Acevedo

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Ab initio metadynamics determination of temperature-dependent free-energy landscape in ultrasmall silver clusters.. <i>Journal of Chemical Physics</i> , 2022 , 156, 154301	3.9	2
47	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	3.9	6
46	Atomic structure and origin of chirality of DNA-stabilized silver clusters. <i>Physical Review Materials</i> , 2020 , 4,	3.2	7
45	Large-Z limit in atoms and solids from first principles. <i>Journal of Chemical Physics</i> , 2019 , 151, 244101	3.9	1
44	Semilocal kinetic energy functionals with parameters from neutral atoms. <i>Physical Review B</i> , 2019 , 100,	3.3	8
43	Silver-Stabilized Guanine Duplex: Structural and Optical Properties. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 4789-4794	6.4	9
42	Optical Properties of Silver-Mediated DNA from Molecular Dynamics and Time Dependent Density Functional Theory. <i>International Journal of Molecular Sciences</i> , 2018 , 19,	6.3	5
41	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	6.4	24
40	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	6.4	12
39	Excitation-dependent fluorescence from atomic/molecular layer deposited sodium-uracil thin films. <i>Scientific Reports</i> , 2017 , 7, 6982	4.9	11
38	Silver-Mediated Double Helix: Structural Parameters for a Robust DNA Building Block. <i>ACS Omega</i> , 2017 , 2, 7343-7348	3.9	19
37	Self-consistent assessment of Englert-Schwinger model on atomic properties. <i>Journal of Chemical Physics</i> , 2017 , 147, 234102	3.9	4
36	Three-Dimensional Uracil Network with Sodium as a Linker. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 26342-26349	3.8	17
35	Structural morphology of carbon nanofibers grown on different substrates. <i>Carbon</i> , 2016 , 98, 343-351	10.4	17
34	Density and localized states impact on amorphous carbon electron transport mechanisms. <i>Journal of Applied Physics</i> , 2016 , 120, 214303	2.5	2
33	Accurate schemes for calculation of thermodynamic properties of liquid mixtures from molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2016 , 145, 244504	3.9	23
32	Silver (I) as DNA glue: Ag(+)-mediated guanine pairing revealed by removing Watson-Crick constraints. <i>Scientific Reports</i> , 2015 , 5, 10163	4.9	101

31	Piezoelectric coefficients and spontaneous polarization of ScAlN. <i>Journal of Physics Condensed Matter</i> , 2015 , 27, 245901	1.8	119
30	Optimizing a parametrized Thomas-Fermi-Dirac-Weizsäcker density functional for atoms. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 31463-71	3.6	11
29	The Role of Hydrogen Bonds in the Stabilization of Silver-Mediated Cytosine Tetramers. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 4061-6	6.4	37
28	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,	6.3	14
27	Optical Spectra of the Special Au ₁₄₄ Gold-Cluster Compounds: Sensitivity to Structure and Symmetry. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 11250-11259	3.8	34
26	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	2.5	9
25	A Multiscale Code for Flexible Hybrid Simulations Using ASE Framework. <i>Computing in Science and Engineering</i> , 2014 , 16, 54-62	1.5	
24	Atomic and electronic structure of tetrahedral amorphous carbon surfaces from density functional theory: Properties and simulation strategies. <i>Carbon</i> , 2014 , 77, 1168-1182	10.4	37
23	Orbital-free density functional theory implementation with the projector augmented-wave method. <i>Journal of Chemical Physics</i> , 2014 , 141, 234102	3.9	58
22	First-Principles Study of Excited State Evolution in a Protected Gold Complex. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 11837-11842	3.8	6
21	Solvent driven formation of silver embedded resorcinarene nanorods. <i>CrystEngComm</i> , 2012 , 14, 347-350	3.3	13
20	Derivatives of the thiolate-protected gold cluster Au ₂₅ (SR) ₁₈ -1. <i>European Physical Journal D</i> , 2011 , 63, 311-314	1.3	12
19	The Al ₅₀ Cp* ₁₂ Cluster: A 138-Electron Closed Shell (L = 6) Superatom. <i>European Journal of Inorganic Chemistry</i> , 2011 , 2011, 2649-2652	2.3	39
18	Electronic and vibrational signatures of the Au ₁₀₂ (p-MBA) ₄₄ cluster. <i>Journal of the American Chemical Society</i> , 2011 , 133, 3752-5	16.4	74
17	Electronic structure of gold, aluminum, and gallium superatom complexes. <i>Physical Review B</i> , 2011 , 84,	3.3	37
16	Evidence of superatom electronic shells in ligand-stabilized aluminum clusters. <i>Journal of Chemical Physics</i> , 2011 , 135, 094701	3.9	40
15	Quantum size effects in ambient CO oxidation catalysed by ligand-protected gold clusters. <i>Nature Chemistry</i> , 2010 , 2, 329-34	17.6	266
14	Theoretical Characterization of Cyclic Thiolated Copper, Silver, and Gold Clusters. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 13571-13576	3.8	46

13	Thiolate-Protected Au ₂₅ Superatoms as Building Blocks: Dimers and Crystals <i>Journal of Physical Chemistry C</i> , 2010 , 114, 15986-15994	3.8	99
12	Experimental and Density Functional Theory Analysis of Serial Introductions of Electron-Withdrawing Ligands into the Ligand Shell of a Thiolate-Protected Au ₂₅ Nanoparticle. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 8276-8281	3.8	59
11	Chirality and electronic structure of the thiolate-protected Au ₃₈ nanocluster. <i>Journal of the American Chemical Society</i> , 2010 , 132, 8210-8	16.4	367
10	Oligomeric Gold-Thiolate Units Define the Properties of the Molecular Junction between Gold and Benzene Dithiols. <i>Journal of Physical Chemistry Letters</i> , 2010 , 1, 1528-1532	6.4	40
9	Electronic structure calculations with GPAW: a real-space implementation of the projector augmented-wave method. <i>Journal of Physics Condensed Matter</i> , 2010 , 22, 253202	1.8	1092
8	Probing the Atomic-Scale Structure of Monolayer-Protected Au ₃₈ Clusters. <i>Microscopy and Microanalysis</i> , 2010 , 16, 1652-1653	0.5	
7	Characterization of iron-carbonyl-protected gold clusters. <i>Journal of the American Chemical Society</i> , 2009 , 131, 12573-5	16.4	17
6	A density functional investigation of thiolate-protected bimetal PdAu ₍₂₄₎ (SR) ₍₁₈₎ (z) clusters: doping the superatom complex. <i>Physical Chemistry Chemical Physics</i> , 2009 , 11, 7123-9	3.6	92
5	Density functional theory based screening of ternary alkali-transition metal borohydrides: a computational material design project. <i>Journal of Chemical Physics</i> , 2009 , 131, 014101	3.9	74
4	Structure and Bonding in the Ubiquitous Icosahedral Metallic Gold Cluster Au ₁₄₄ (SR) ₆₀ . <i>Journal of Physical Chemistry C</i> , 2009 , 113, 5035-5038	3.8	363
3	A unified view of ligand-protected gold clusters as superatom complexes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008 , 105, 9157-62	11.5	1264
2	Conductance through atomic point contacts between fcc(100) electrodes of gold. <i>European Physical Journal B</i> , 2008 , 66, 497-501	1.2	1
1	Quantum walks on Cayley graphs. <i>Journal of Physics A</i> , 2006 , 39, 585-599		18