Olga Lopez-Acevedo

List of Publications by Year
in descending order

48 papers	5,578 citations	279798 23 h-index	197818 49 g-index
50 all docs	50 docs citations	50 times ranked	5904 citing authors

#	Article	IF	Citations
1	Ab initio metadynamics determination of temperature-dependent free-energy landscape in ultrasmall silver clusters. Journal of Chemical Physics, 2022, 156, 154301.	3.0	4
2	Real-time time-dependent density functional theory implementation of electronic circular dichroism applied to nanoscale metalâ€“organic clusters. Journal of Chemical Physics, 2021, 154, 114102.	3.0	16
3	Atomic structure and origin of chirality of DNA-stabilized silver clusters. Physical Review Materials, 2020, 4, .	2.4	13
4	Large-Z limit in atoms and solids from first principles. Journal of Chemical Physics, 2019, 151, 244101.	3.0	2
5	Semilocal kinetic energy functionals with parameters from neutral atoms. Physical Review B, 2019, 100, .	3.2	10
6	Silver-Stabilized Guanine Duplex: Structural and Optical Properties. Journal of Physical Chemistry Letters, 2018, 9, 4789-4794.	4.6	15
7	Optical Properties of Silver-Mediated DNA from Molecular Dynamics and Time Dependent Density Functional Theory. International Journal of Molecular Sciences, 2018, 19, 2346.	4.1	7
8	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.	5.3	32
9	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.	5.3	18
10	Excitation-dependent fluorescence from atomic/molecular layer deposited sodium-uracil thin films. Scientific Reports, 2017, 7, 6982.	3.3	13
11	Silver-Mediated Double Helix: Structural Parameters for a Robust DNA Building Block. ACS Omega, 2017, 2, 7343-7348.	3.5	26
12	Self-consistent assessment of Englert-Schwinger model on atomic properties. Journal of Chemical Physics, 2017, 147, 234102.	3.0	4
13	Density and localized states' impact on amorphous carbon electron transport mechanisms. Journal of Applied Physics, 2016, 120, 214303.	2.5	3
14	Accurate schemes for calculation of thermodynamic properties of liquid mixtures from molecular dynamics simulations. Journal of Chemical Physics, 2016, 145, 244504.	3.0	38
15	Three-Dimensional Uracil Network with Sodium as a Linker. Journal of Physical Chemistry C, 2016, 120, 26342-26349.	3.1	18
16	Structural morphology of carbon nanofibers grown on different substrates. Carbon, 2016, 98, 343-351.	10.3	25
17	The Role of Hydrogen Bonds in the Stabilization of Silver-Mediated Cytosine Tetramers. Journal of Physical Chemistry Letters, 2015, 6, 4061-4066.	4.6	43
18	On the interaction between gold and silver metal atoms and DNA/RNA nucleobases â€“ a comprehensive computational study of ground state properties. Nanotechnology Reviews, 2015, 4, 173-191.	5.8	23

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19	Optical Spectra of the Special Au₁₄₄ Gold-Cluster Compounds: Sensitivity to Structure and Symmetry. Journal of Physical Chemistry C, 2015, 119, 11250-11259.	3.1	37
20	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
21	Silver (I) as DNA glue: Ag+-mediated guanine pairing revealed by removing Watson-Crick constraints. Scientific Reports, 2015, 5, 10163.	3.3	127
22	Piezoelectric coefficients and spontaneous polarization of ScAlN. Journal of Physics Condensed Matter, 2015, 27, 245901.	1.8	209
23	Optimizing a parametrized Thomasâ€“Fermiâ€“Diracâ€“WeizsÃcker density functional for atoms. Physical Chemistry Chemical Physics, 2015, 17, 31463-31471.	2.8	16
24	Orbital-free density functional theory implementation with the projector augmented-wave method. Journal of Chemical Physics, 2014, 141, 234102.	3.0	74
25	A Multiscale Code for Flexible Hybrid Simulations Using ASE Framework. Computing in Science and Engineering, 2014, 16, 54-62.	1.2	4
26	Atomic and electronic structure of tetrahedral amorphous carbon surfaces from density functional theory: Properties and simulation strategies. Carbon, 2014, 77, 1168-1182.	10.3	41
27	First-Principles Study of Excited State Evolution in a Protected Gold Complex. Journal of Physical Chemistry C, 2013, 117, 11837-11842.	3.1	6
28	Solvent driven formation of silver embedded resorcinarene nanorods. CrystEngComm, 2012, 14, 347-350.	2.6	13
29	Electronic and Vibrational Signatures of the Au₁₀₂(p-MBA)₄₄ Cluster. Journal of the American Chemical Society, 2011, 133, 3752-3755.	13.7	80
30	Derivatives of the thiolate-protected gold cluster Au25(SR)18 -1. European Physical Journal D, 2011, 63, 311-314.	1.3	13
31	The Al50Cp*12 Cluster - A 138-Electron Closed Shell (L = 6) Superatom. European Journal of Inorganic Chemistry, 2011, 2011, 2649-2652.	2.0	41
32	Electronic structure of gold, aluminum, and gallium superatom complexes. Physical Review B, 2011, 84, .	3.2	39
33	Evidence of superatom electronic shells in ligand-stabilized aluminum clusters. Journal of Chemical Physics, 2011, 135, 094701.	3.0	42
34	Probing the Atomic-Scale Structure of Monolayer-Protected Au38 Clusters. Microscopy and Microanalysis, 2010, 16, 1652-1653.	0.4	0
35	Quantum size effects in ambient CO oxidation catalysed by ligand-protected gold clusters. Nature Chemistry, 2010, 2, 329-334.	13.6	295
36	Theoretical Characterization of Cyclic Thiolated Copper, Silver, and Gold Clusters. Journal of Physical Chemistry C, 2010, 114, 13571-13576.	3.1	51

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37	Thiolate-Protected Au₂₅ Superatoms as Building Blocks: Dimers and Crystals. Journal of Physical Chemistry C, 2010, 114, 15986-15994.	3.1	109
38	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.	3.1	61
39	Chirality and Electronic Structure of the Thiolate-Protected Au₃₈ Nanocluster. Journal of the American Chemical Society, 2010, 132, 8210-8218.	13.7	401
40	Oligomeric Goldâ^'Thiolate Units Define the Properties of the Molecular Junction between Gold and Benzene Dithiols. Journal of Physical Chemistry Letters, 2010, 1, 1528-1532.	4.6	43
41	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	1,451
42	Characterization of Ironâ^'Carbonyl-Protected Gold Clusters. Journal of the American Chemical Society, 2009, 131, 12573-12575.	13.7	17
43	A density functional investigation of thiolate-protected bimetal PdAu24(SR)18z clusters: doping the superatom complex. Physical Chemistry Chemical Physics, 2009, 11, 7123.	2.8	100
44	Density functional theory based screening of ternary alkali-transition metal borohydrides: A computational material design project. Journal of Chemical Physics, 2009, 131, 014101.	3.0	77
45	Structure and Bonding in the Ubiquitous Icosahedral Metallic Gold Cluster Au₁₄₄(SR)₆₀. Journal of Physical Chemistry C, 2009, 113, 5035-5038.	3.1	393
46	Conductance through atomic point contacts between fcc(100) electrodes of gold. European Physical Journal B, 2008, 66, 497-501.	1.5	1
47	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.	7.1	1,472
48	Quantum walks on Cayley graphs. Journal of Physics A, 2006, 39, 585-599.	1.6	23