Jaakko Akola

List of Publications by Citations

Source: https://exaly.com/author-pdf/1934604/jaakko-akola-publications-by-citations.pdf
Version: 2024-04-09

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.
The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

111 papers	6,411 citations	38 h-index	79 g-index
124 ext. papers	7,055 ext. citations	5.5 avg, IF	5.83 L-index

#	Paper	IF	Citations
111	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
110	On the structure of thiolate-protected Au25. *Journal of the American Chemical Society*, **2008**, 130, 3756-7	16.4	639
109	Structural phase transitions on the nanoscale: The crucial pattern in the phase-change materials Ge2Sb2Te5 and GeTe. *Physical Review B*, **2007**, 76,	3.3	373
108	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
107	Quantum size effects in ambient CO oxidation catalysed by ligand-protected gold clusters. *Nature Chemistry*, **2010**, 2, 329-34	17.6	266
106	Photoelectron spectra of aluminum cluster anions: Temperature effects and ab initio simulations. *Physical Review B*, **1999**, 60, R11297-R11300	3.3	247
105	From local structure to nanosecond recrystallization dynamics in AgInSbTe phase-change materials. *Nature Materials*, **2011**, 10, 129-34	27	204
104	Ionization potential of aluminum clusters. *Physical Review B*, **1998**, 58, 3601-3604	3.3	106
103	Aluminum cluster anions: Photoelectron spectroscopy and ab initio simulations. *Physical Review B*, **2000**, 62, 13216-13228	3.3	105
102	Binary alloys of Ge and Te: order, voids, and the eutectic composition. *Physical Review Letters*, **2008**, 100, 205502	7.4	103
101	Thiolate-Protected Au25 Superatoms as Building Blocks: Dimers and Crystals *Journal of Physical Chemistry C*, **2010**, 114, 15986-15994	3.8	99
100	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
99	Edge-dependent selection rules in magic triangular graphene flakes. *Physical Review B*, **2008**, 77,	3.3	90
98	Density functional study of amorphous, liquid and crystalline Ge(2)Sb(2)Te(5): homopolar bonds and/or AB alternation?. *Journal of Physics Condensed Matter*, **2008**, 20, 465103	1.8	88
97	Density functional study of alkali-metal atoms and monolayers on graphite (0001). *Physical Review B*, **2007**, 75,	3.3	87
96	ATP Hydrolysis in Water A Density Functional Study. *Journal of Physical Chemistry B*, **2003**, 107, 11774-11783	3.4	86
95	Relationship between topological order and glass forming ability in densely packed enstatite and forsterite composition glasses. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 14780-5	11.5	81

94	Atomistic Simulations of Functional Au144(SR)60 Gold Nanoparticles in Aqueous Environment. *Journal of Physical Chemistry C*, **2012**, 116, 9805-9815	3.8	80
93	Electronic structure of triangular, hexagonal and round graphene flakes near the Fermi level. *New Journal of Physics*, **2008**, 10, 103015	2.9	78
92	Experimentally constrained density-functional calculations of the amorphous structure of the prototypical phase-change material Ge2Sb2Te5. *Physical Review B*, **2009**, 80,	3.3	73
91	Nucleus-driven crystallization of amorphous Ge2Sb2Te5: A density functional study. *Physical Review B*, **2012**, 86,	3.3	66
90	Polymorphism in phase-change materials: melt-quenched and as-deposited amorphous structures in Ge2Sb2Te5 from density functional calculations. *Physical Review B*, **2011**, 83,	3.3	64
89	Thermal expansion in small metal clusters and its impact on the electric polarizability. *Physical Review Letters*, **2000**, 84, 3827-30	7.4	61
88	Cationic Au Nanoparticle Binding with Plasma Membrane-like Lipid Bilayers: Potential Mechanism for Spontaneous Permeation to Cells Revealed by Atomistic Simulations. *Journal of Physical Chemistry C*, **2014**, 118, 11131-11141	3.8	60
87	Lead silicate glasses: Binary network-former glasses with large amounts of free volume. *Physical Review B*, **2010**, 82,	3.3	60
86	Highly ductile amorphous oxide at room temperature and high strain rate. *Science*, **2019**, 366, 864-869	33.3	58
85	Molecular-Scale Ligand Effects in Small Gold-Thiolate Nanoclusters. *Journal of the American Chemical Society*, **2018**, 140, 15430-15436	16.4	56
84	Structure of amorphous Ge8Sb2Te11: GeTe-Sb2Te3 alloys and optical storage. *Physical Review B*, **2009**, 79,	3.3	53
83	On the Structure of a Thiolated Gold Cluster: Au44(SR)282 *Journal of Physical Chemistry C*, **2010**, 114, 15883-15889	3.8	53
82	Simulation of crystallization in Ge2Sb2Te5: A memory effect in the canonical phase-change material. *Physical Review B*, **2014**, 90,	3.3	51
81	Atomic and electronic structures of an extremely fragile liquid. *Nature Communications*, **2014**, 5, 5892	17.4	51
80	Metallic evolution of small magnesium clusters. *European Physical Journal D*, **2001**, 16, 21-24	1.3	45
79	Network topology for the formation of solvated electrons in binary CaO-Al2O3 composition glasses. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 10129-34	11.5	42
78	Crystallization processes in the phase change material Ge2Sb2Te5: Unbiased density functional/molecular dynamics simulations. *Physical Review B*, **2016**, 94,	3.3	40
77	Atomistic simulations of anionic Au144(SR)60 nanoparticles interacting with asymmetric model lipid membranes. *Biochimica Et Biophysica Acta - Biomembranes*, **2014**, 1838, 2852-60	3.8	40

76	Density variations in liquid tellurium: Roles of rings, chains, and cavities. *Physical Review B*, **2010**, 81,	3.3	40
75	Structure and dynamics in amorphous tellurium and Ten clusters: A density functional study. *Physical Review B*, **2012**, 85,	3.3	40
74	Amorphous Ge□Te□density functional, high-energy x-ray and neutron diffraction study. *Journal of Physics Condensed Matter*, **2012**, 24, 015802	1.8	38
73	Density functional study of gold atoms and clusters on a graphite (0001) surface with defects. *Physical Review B*, **2006**, 74,	3.3	38
72	Structure, electronic, and vibrational properties of glassy Ga11Ge11Te78: Experimentally constrained density functional study. *Physical Review B*, **2012**, 86,	3.3	36
71	Role of the Central Gold Atom in Ligand-Protected Biicosahedral Au24 and Au25 Clusters. *Journal of Physical Chemistry C*, **2013**, 117, 22079-22086	3.8	34
70	Sodium atoms and clusters on graphite by density functional theory. *Physical Review B*, **2004**, 69,	3.3	31
69	First-principles simulations of hydrogen peroxide formation catalyzed by small neutral gold clusters. *Physical Chemistry Chemical Physics*, **2009**, 11, 6359-64	3.6	29
68	Coexisting Honeycomb and Kagome Characteristics in the Electronic Band Structure of Molecular Graphene. *Nano Letters*, **2016**, 16, 3519-23	11.5	29
67	Geometric Structure and Chemical Ordering of Large AuCu Clusters: A Computational Study. *Journal of Physical Chemistry C*, **2017**, 121, 10809-10816	3.8	28
66	Regeneration of sulfur-poisoned Pd-based catalyst for natural gas oxidation. *Journal of Catalysis*, **2018**, 358, 253-265	7.3	26
65	Density functional calculations of ATP systems. 2. ATP hydrolysis at the active site of actin. *Journal of Physical Chemistry B*, **2006**, 110, 8121-9	3.4	25
64	Amorphous structures of Ge/Sb/Te alloys: Density functional simulations. *Physica Status Solidi (B): Basic Research*, **2012**, 249, 1851-1860	1.3	24
63	Ultrahigh-pressure form of SiO2 glass with dense pyrite-type crystalline homology. *Physical Review B*, **2019**, 99,	3.3	23
62	The Role of Temperature and Lipid Charge on Intake/Uptake of Cationic Gold Nanoparticles into Lipid Bilayers. *Small*, **2019**, 15, e1805046	11	22
61	Interaction of Au16 Nanocluster with Defects in Supporting Graphite: A Density-Functional Study. *Journal of Physical Chemistry C*, **2011**, 115, 15240-15250	3.8	22
60	Proton Distribution and Dynamics in Y- and Zn-Doped BaZrO3. *Journal of Physical Chemistry C*, **2014** , 118, 18846-18852	3.8	21
59	Structure of liquid phase change material AgInSbTe from density functional/molecular dynamics simulations. *Applied Physics Letters*, **2009**, 94, 251905	3.4	21

58	CLEASE: a versatile and user-friendly implementation of cluster expansion method. *Journal of Physics Condensed Matter*, **2019**, 31, 325901	1.8	20
57	Electronic properties of single-walled carbon nanotubes inside cyclic supermolecules. *Journal of Physical Chemistry B*, **2006**, 110, 5186-90	3.4	20
56	How do Water Solvent and Glutathione Ligands Affect the Structure and Electronic Properties of Au25(SR)18(-)?. *Journal of Physical Chemistry Letters*, **2015**, 6, 3859-65	6.4	19
55	Structure and properties of densified silica glass: characterizing the order within disorder. *NPG Asia Materials*, **2020**, 12,	10.3	19
54	CO oxidation catalyzed by neutral and anionic Cu20 clusters: relationship between charge and activity. *Physical Chemistry Chemical Physics*, **2015**, 17, 7067-76	3.6	18
53	Steered molecular dynamics simulations of ligand-receptor interaction in lipocalins. *European Biophysics Journal*, **2011**, 40, 181-94	1.9	18
52	Synergistic Computational–Experimental Discovery of Highly Selective PtCu Nanocluster Catalysts for Acetylene Semihydrogenation. *ACS Catalysis*, **2020**, 10, 451-457	13.1	18
51	Structure and dynamics in liquid bismuth and Bi(n) clusters: a density functional study. *Journal of Chemical Physics*, **2014**, 141, 194503	3.9	17
50	Bright beaches of nanoscale potassium islands on graphite in STM imaging. *Physical Review Letters*, **2009**, 102, 106102	7.4	17
49	Heating of Al13 and Al14 clusters. *Physical Review B*, **2001**, 63,	3.3	17
48	Densified low-hygroscopic form of P2O5 glass. *Journal of Materials Chemistry*, **2011**, 21, 10442		16
47	Catalytic Activity of AuCu Clusters on MgO(100): Effect of Alloy Composition for CO Oxidation. *Journal of Physical Chemistry C*, **2017**, 121, 10876-10886	3.8	15
46	CO Oxidation on the Au15Cu15 Cluster and the Role of Vacancies in the MgO(100) Support. *Journal of Physical Chemistry C*, **2016**, 120, 26747-26758	3.8	15
45	Crystallization of supercooled liquid antimony: A density functional study. *Physical Review B*, **2017**, 96,	3.3	15
44	Density functional calculations of ATP systems. 1. Crystalline ATP hydrates and related molecules. *Journal of Physical Chemistry B*, **2006**, 110, 8110-20	3.4	14
43	Close packing of clusters: Application to Al100. *Physical Review B*, **2003**, 68,	3.3	14
42	Combined experimental and theoretical study of acetylene semi-hydrogenation over Pd/Al2O3. *International Journal of Hydrogen Energy*, **2020**, 45, 1283-1296	6.7	14
41	Structure, electronic, and vibrational properties of amorphous AsS2 and AgAsS2: Experimentally constrained density functional study. *Physical Review B*, **2014**, 89,	3.3	13

40	Electronic shell and supershell structure in graphene flakes. *European Physical Journal D*, **2009**, 52, 143-146	1.3	13
39	Temperature-dependent ionization potential of sodium clusters. *European Physical Journal D*, **2000**, 8, 93-99	1.3	13
38	The electrooxidation-induced structural changes of gold di-superatomic molecules: Au23vs. Au25. *Physical Chemistry Chemical Physics*, **2016**, 18, 4822-7	3.6	12
37	Speeding up crystallization. *Science*, **2017**, 358, 1386	33.3	12
36	Aluminum-lithium clusters: First-principles simulation of geometries and electronic properties. *Physical Review B*, **2002**, 65,	3.3	12
35	Conductivity control via minimally invasive anti-Frenkel defects in a functional oxide. *Nature Materials*, **2020**, 19, 1195-1200	27	12
34	Collective excitations and viscosity in liquid Bi. *Journal of Chemical Physics*, **2016**, 145, 184502	3.9	12
33	Structure of amorphous Ag/Ge/S alloys: experimentally constrained density functional study. *Journal of Physics Condensed Matter*, **2015**, 27, 485304	1.8	11
32	The molecular mechanism of the ligand exchange reaction of an antibody against a glutathione-coated gold cluster. *Nanoscale*, **2017**, 9, 3121-3127	7.7	10
31	Density functional study of Cu(2+)-phenylalanine complex under micro-solvation environment. *Journal of Molecular Graphics and Modelling*, **2013**, 45, 180-91	2.8	10
30	Density functional simulations of structure and polymorphism in Ga/Sb films. *Journal of Physics Condensed Matter*, **2013**, 25, 115801	1.8	10
29	Branching Reactions in Polycarbonate: A Density Functional Study. *Macromolecules*, **2003**, 36, 1355-1360	5.5	10
28	Strain-engineered widely tunable perfect absorption angle in black phosphorus from first principles. *Physical Review B*, **2020**, 102,	3.3	10
27	Real-space Wigner-Seitz cells imaging of potassium on graphite via elastic atomic manipulation. *Scientific Reports*, **2015**, 5, 8276	4.9	8
26	Precipitate formation in aluminium alloys: Multi-scale modelling approach. *Acta Materialia*, **2020**, 195, 123-131	8.4	8
25	Silver Sulfide Nanoclusters and the Superatom Model. *Journal of Physical Chemistry C*, **2015**, 119, 1583-1590	4.8	8
24	The structure of MgO-SiO2 glasses at elevated pressure. *Journal of Physics Condensed Matter*, **2012**, 24, 225403	1.8	8
23	Very sharp diffraction peak in nonglass-forming liquid with the formation of distorted tetraclusters. *NPG Asia Materials*, **2020**, 12,	10.3	7

22	Density functional study of structure and dynamics in liquid antimony and Sb clusters. *Journal of Chemical Physics*, **2017**, 146, 194502	3.9	7
21	Density-functional investigation of molecular graphene: CO on Cu(111). *Physical Review B*, **2014**, 90,	3.3	7
20	Ionization potential of Al6 and Al7 as a function of temperature. *European Physical Journal D*, **1999**, 9, 179-182	1.3	7
19	Atomistic simulations of early stage clusters in AlMg alloys. *Acta Materialia*, **2019**, 166, 484-492	8.4	7
18	Varying oxygen coverage on Cu and its effect on CO oxidation. *Physical Chemistry Chemical Physics*, **2019**, 21, 11351-11358	3.6	4
17	Simple metal under tensile stress: layer-dependent herringbone reconstruction of thin potassium films on graphite. *Scientific Reports*, **2015**, 5, 10165	4.9	4
16	Superatom Model for Ag Nanocluster with Delocalized Electrons. *Journal of Physical Chemistry C*, **2015**, 119, 21165-21172	3.8	4
15	Tuning electronic properties of graphene heterostructures by amorphous-to-crystalline phase transitions. *Physical Review B*, **2016**, 93,	3.3	4
14	DFT simulations and microkinetic modelling of 1-pentyne hydrogenation on Cu20 model catalysts. *Journal of Molecular Graphics and Modelling*, **2016**, 65, 61-70	2.8	4
13	Improving the Adsorption of Au Atoms and Nanoparticles on Graphite via Li Intercalation. *Journal of Physical Chemistry C*, **2013**, 117, 22683-22695	3.8	4
12	Comment on "Formation of large voids in the amorphous phase-change memory Ge2Sb2Te5 alloy". *Physical Review Letters*, **2010**, 104, 019603; author replly 019604	7.4	4
11	Publisher Note: Experimentally constrained density-functional calculations of the amorphous structure of the prototypical phase-change material Ge2Sb2Te5 [Phys. Rev. B 80, 020201(R) (2009)]. *Physical Review B*, **2009**, 80,	3.3	4
10	Reactions of Polycarbonate with Cyclohexene Oxide and Phosphites: A Density Functional Study. *Macromolecules*, **2002**, 35, 2327-2334	5.5	4
9	Comparison of optical response from DFT random phase approximation and a low-energy effective model: Strained phosphorene. *Physical Review B*, **2021**, 104,	3.3	3
8	Nanoparticle Membrane Interactions: The Role of Temperature and Lipid Charge on Intake/Uptake of Cationic Gold Nanoparticles into Lipid Bilayers (Small 23/2019). *Small*, **2019**, 15, 1970124	11	2
7	Josephson effect in graphene bilayers with adjustable relative displacement. *Physical Review Research*, **2020**, 2,	3.9	2
6	Density functional and classical simulations of liquid and glassy selenium. *Physical Review B*, **2020**, 102,	3.3	2
5	Electric-field-induced annihilation of localized gap defect states in amorphous phase-change memory materials. *Acta Materialia*, **2021**, 223, 117465	8.4	1

4	Training sets based on uncertainty estimates in the cluster-expansion method. *JPhys Energy*, **2021**, 3, 034012	4.9	1
3	Ring-Opening and Branching in Polycarbonates: A Density Functional-Monte Carlo Study. *ACS Symposium Series*, **2005**, 200-213	0.4	
2	Ionization potential of Al6 and A17 as a function of temperature **1999**, 179-182		
1	The Prototype Phase Change Material ({mathrm{Ge}_2}{mathrm{Sb}_2}{mathrm{Te}_5}): Amorphous Structure and Crystallization. *Springer Series in Materials Science*, **2015**, 457-484	0.9	