Jaakko Akola

List of Publications by Year in Descending Order

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	Electric-field-induced annihilation of localized gap defect states in amorphous phase-change memory materials. *Acta Materialia*, **2021**, 223, 117465	8.4	1
110	Training sets based on uncertainty estimates in the cluster-expansion method. *JPhys Energy*, **2021**, 3, 034012	4.9	1
109	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
108	Precipitate formation in aluminium alloys: Multi-scale modelling approach. *Acta Materialia*, **2020**, 195, 123-131	8.4	8
107	Very sharp diffraction peak in nonglass-forming liquid with the formation of distorted tetraclusters. *NPG Asia Materials*, **2020**, 12,	10.3	7
106	Josephson effect in graphene bilayers with adjustable relative displacement. *Physical Review Research*, **2020**, 2,	3.9	2
105	Structure and properties of densified silica glass: characterizing the order within disorder. *NPG Asia Materials*, **2020**, 12,	10.3	19
104	Synergistic Computational–Experimental Discovery of Highly Selective PtCu Nanocluster Catalysts for Acetylene Semihydrogenation. *ACS Catalysis*, **2020**, 10, 451-457	13.1	18
103	Strain-engineered widely tunable perfect absorption angle in black phosphorus from first principles. *Physical Review B*, **2020**, 102,	3.3	10
102	Density functional and classical simulations of liquid and glassy selenium. *Physical Review B*, **2020**, 102,	3.3	2
101	Conductivity control via minimally invasive anti-Frenkel defects in a functional oxide. *Nature Materials*, **2020**, 19, 1195-1200	27	12
100	Combined experimental and theoretical study of acetylene semi-hydrogenation over Pd/Al2O3. *International Journal of Hydrogen Energy*, **2020**, 45, 1283-1296	6.7	14
99	Ultrahigh-pressure form of SiO2 glass with dense pyrite-type crystalline homology. *Physical Review B*, **2019**, 99,	3.3	23
98	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
97	Varying oxygen coverage on Cu and its effect on CO oxidation. *Physical Chemistry Chemical Physics*, **2019**, 21, 11351-11358	3.6	4
96	The Role of Temperature and Lipid Charge on Intake/Uptake of Cationic Gold Nanoparticles into Lipid Bilayers. *Small*, **2019**, 15, e1805046	11	22
95	CLEASE: a versatile and user-friendly implementation of cluster expansion method. *Journal of Physics Condensed Matter*, **2019**, 31, 325901	1.8	20

94	Highly ductile amorphous oxide at room temperature and high strain rate. *Science*, **2019**, 366, 864-869	33.3	58
93	Atomistic simulations of early stage clusters in AlMg alloys. *Acta Materialia*, **2019**, 166, 484-492	8.4	7
92	Regeneration of sulfur-poisoned Pd-based catalyst for natural gas oxidation. *Journal of Catalysis*, **2018**, 358, 253-265	7.3	26
91	Molecular-Scale Ligand Effects in Small Gold-Thiolate Nanoclusters. *Journal of the American Chemical Society*, **2018**, 140, 15430-15436	16.4	56
90	Geometric Structure and Chemical Ordering of Large AuCu Clusters: A Computational Study. *Journal of Physical Chemistry C*, **2017**, 121, 10809-10816	3.8	28
89	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
88	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
87	Speeding up crystallization. *Science*, **2017**, 358, 1386	33.3	12
86	Crystallization of supercooled liquid antimony: A density functional study. *Physical Review B*, **2017**, 96,	3.3	15
85	Density functional study of structure and dynamics in liquid antimony and Sb clusters. *Journal of Chemical Physics*, **2017**, 146, 194502	3.9	7
84	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
83	Tuning electronic properties of graphene heterostructures by amorphous-to-crystalline phase transitions. *Physical Review B*, **2016**, 93,	3.3	4
82	Crystallization processes in the phase change material Ge2Sb2Te5: Unbiased density functional/molecular dynamics simulations. *Physical Review B*, **2016**, 94,	3.3	40
81	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
80	The electrooxidation-induced structural changes of gold di-superatomic molecules: Au23vs. Au25. *Physical Chemistry Chemical Physics*, **2016**, 18, 4822-7	3.6	12
79	Collective excitations and viscosity in liquid Bi. *Journal of Chemical Physics*, **2016**, 145, 184502	3.9	12
78	Coexisting Honeycomb and Kagome Characteristics in the Electronic Band Structure of Molecular Graphene. *Nano Letters*, **2016**, 16, 3519-23	11.5	29
77	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

76	Real-space Wigner-Seitz cells imaging of potassium on graphite via elastic atomic manipulation. *Scientific Reports*, **2015**, 5, 8276	4.9	8
75	Simple metal under tensile stress: layer-dependent herringbone reconstruction of thin potassium films on graphite. *Scientific Reports*, **2015**, 5, 10165	4.9	4
74	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
73	Superatom Model for Ag_{8} Nanocluster with Delocalized Electrons. *Journal of Physical Chemistry C*, **2015**, 119, 21165-21172	3.8	4
72	Structure of amorphous Ag/Ge/S alloys: experimentally constrained density functional study. *Journal of Physics Condensed Matter*, **2015**, 27, 485304	1.8	11
71	Silver Sulfide Nanoclusters and the Superatom Model. *Journal of Physical Chemistry C*, **2015**, 119, 1583-1590	3.8	8
70	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	
69	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
68	Proton Distribution and Dynamics in Y- and Zn-Doped BaZrO3. *Journal of Physical Chemistry C*, **2014** , 118, 18846-18852	3.8	21
67	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
66	Simulation of crystallization in Ge2Sb2Te5: A memory effect in the canonical phase-change material. *Physical Review B*, **2014**, 90,	3.3	51
65	Density-functional investigation of molecular graphene: CO on Cu(111). *Physical Review B*, **2014**, 90,	3.3	7
64	Structure, electronic, and vibrational properties of amorphous AsS2 and AgAsS2: Experimentally constrained density functional study. *Physical Review B*, **2014**, 89,	3.3	13
63	Atomic and electronic structures of an extremely fragile liquid. *Nature Communications*, **2014**, 5, 5892	17.4	51
62	Structure and dynamics in liquid bismuth and Bi(n) clusters: a density functional study. *Journal of Chemical Physics*, **2014**, 141, 194503	3.9	17
61	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
60	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
59	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

58	Density functional simulations of structure and polymorphism in Ga/Sb films. *Journal of Physics Condensed Matter*, **2013**, 25, 115801	1.8	10
57	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
56	Amorphous structures of Ge/Sb/Te alloys: Density functional simulations. *Physica Status Solidi (B): Basic Research*, **2012**, 249, 1851-1860	1.3	24
55	Atomistic Simulations of Functional Au144(SR)60 Gold Nanoparticles in Aqueous Environment. *Journal of Physical Chemistry C*, **2012**, 116, 9805-9815	3.8	80
54	The structure of MgO-SiO2 glasses at elevated pressure. *Journal of Physics Condensed Matter*, **2012**, 24, 225403	1.8	8
53	Structure and dynamics in amorphous tellurium and Ten clusters: A density functional study. *Physical Review B*, **2012**, 85,	3.3	40
52	Nucleus-driven crystallization of amorphous Ge2Sb2Te5: A density functional study. *Physical Review B*, **2012**, 86,	3.3	66
51	Structure, electronic, and vibrational properties of glassy Ga11Ge11Te78: Experimentally constrained density functional study. *Physical Review B*, **2012**, 86,	3.3	36
50	Amorphous Ge□Te□density functional, high-energy x-ray and neutron diffraction study. *Journal of Physics Condensed Matter*, **2012**, 24, 015802	1.8	38
49	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
48	From local structure to nanosecond recrystallization dynamics in AgInSbTe phase-change materials. *Nature Materials*, **2011**, 10, 129-34	27	204
47	Steered molecular dynamics simulations of ligand-receptor interaction in lipocalins. *European Biophysics Journal*, **2011**, 40, 181-94	1.9	18
46	Densified low-hygroscopic form of P2O5 glass. *Journal of Materials Chemistry*, **2011**, 21, 10442		16
45	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
44	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
43	Quantum size effects in ambient CO oxidation catalysed by ligand-protected gold clusters. *Nature Chemistry*, **2010**, 2, 329-34	17.6	266
42	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
41	Density variations in liquid tellurium: Roles of rings, chains, and cavities. *Physical Review B*, **2010**, 81,	3.3	40

40	Thiolate-Protected Au25 Superatoms as Building Blocks: Dimers and Crystals *Journal of Physical Chemistry C*, **2010**, 114, 15986-15994	3.8	99
39	Lead silicate glasses: Binary network-former glasses with large amounts of free volume. *Physical Review B*, **2010**, 82,	3.3	60
38	On the Structure of a Thiolated Gold Cluster: Au44(SR)282 *Journal of Physical Chemistry C*, **2010**, 114, 15883-15889	3.8	53
37	Publisher's 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
36	Structure of amorphous Ge8Sb2Te11: GeTe-Sb2Te3 alloys and optical storage. *Physical Review B*, **2009**, 79,	3.3	53
35	Bright beaches of nanoscale potassium islands on graphite in STM imaging. *Physical Review Letters*, **2009**, 102, 106102	7.4	17
34	Structure of liquid phase change material AgInSbTe from density functional/molecular dynamics simulations. *Applied Physics Letters*, **2009**, 94, 251905	3.4	21
33	Experimentally constrained density-functional calculations of the amorphous structure of the prototypical phase-change material Ge2Sb2Te5. *Physical Review B*, **2009**, 80,	3.3	73
32	Electronic shell and supershell structure in graphene flakes. *European Physical Journal D*, **2009**, 52, 143-146	1.9	13
31	First-principles simulations of hydrogen peroxide formation catalyzed by small neutral gold clusters. *Physical Chemistry Chemical Physics*, **2009**, 11, 6359-64	3.6	29
30	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
29	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
28	On the structure of thiolate-protected Au25. *Journal of the American Chemical Society*, **2008**, 130, 3756-7	16.4	639
27	Electronic structure of triangular, hexagonal and round graphene flakes near the Fermi level. *New Journal of Physics*, **2008**, 10, 103015	2.9	78
26	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
25	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
24	Binary alloys of Ge and Te: order, voids, and the eutectic composition. *Physical Review Letters*, **2008**, 100, 205502	7.4	103
23	Edge-dependent selection rules in magic triangular graphene flakes. *Physical Review B*, **2008**, 77,	3.3	90

22	Density functional study of alkali-metal atoms and monolayers on graphite (0001). *Physical Review B*, **2007**, 75,	3.3	87
21	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
20	Electronic properties of single-walled carbon nanotubes inside cyclic supermolecules. *Journal of Physical Chemistry B*, **2006**, 110, 5186-90	3.4	20
19	Density functional study of gold atoms and clusters on a graphite (0001) surface with defects. *Physical Review B*, **2006**, 74,	3.3	38
18	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
17	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
16	Ring-Opening and Branching in Polycarbonates: A Density Functional-Monte Carlo Study. *ACS Symposium Series*, **2005**, 200-213	0.4	
15	Sodium atoms and clusters on graphite by density functional theory. *Physical Review B*, **2004**, 69,	3.3	31
14	ATP Hydrolysis in Water A Density Functional Study. *Journal of Physical Chemistry B*, **2003**, 107, 11774-11783	3.4	86
13	Branching Reactions in Polycarbonate: A Density Functional Study. *Macromolecules*, **2003**, 36, 1355-1360	5.5	10
12	Close packing of clusters: Application to Al100. *Physical Review B*, **2003**, 68,	3.3	14
11	Aluminum-lithium clusters: First-principles simulation of geometries and electronic properties. *Physical Review B*, **2002**, 65,	3.3	12
10	Reactions of Polycarbonate with Cyclohexene Oxide and Phosphites:A Density Functional Study. *Macromolecules*, **2002**, 35, 2327-2334	5.5	4
9	Metallic evolution of small magnesium clusters. *European Physical Journal D*, **2001**, 16, 21-24	1.3	45
8	Heating of Al13and Al14 clusters. *Physical Review B*, **2001**, 63,	3.3	17
7	Temperature-dependent ionization potential of sodium clusters. *European Physical Journal D*, **2000**, 8, 93-99	1.3	13
6	Aluminum cluster anions: Photoelectron spectroscopy and ab initio simulations. *Physical Review B*, **2000**, 62, 13216-13228	3.3	105
5	Thermal expansion in small metal clusters and its impact on the electric polarizability. *Physical Review Letters*, **2000**, 84, 3827-30	7.4	61

4	Photoelectron spectra of aluminum cluster anions: Temperature effects and ab initio simulations. *Physical Review B*, **1999**, 60, R11297-R11300	3.3	247
3	Ionization potential of Al6 and Al7 as a function of temperature. *European Physical Journal D*, **1999**, 9, 179-182	1.3	7
2	Ionization potential of Al6 and A17 as a function of temperature **1999**, 179-182		
1	Ionization potential of aluminum clusters. *Physical Review B*, **1998**, 58, 3601-3604	3.3	106