Kari Laasonen

List of Publications by Year in Descending Order

51 papers	4,702 citations	31 h-index	51 g-index
51 ext. papers	5,000 ext. citations	5.3 avg, IF	5.29 L-index

#	Paper	IF	Citations
51	Designing of low Pt electrocatalyst through immobilization on metal@C support for efficient hydrogen evolution reaction in acidic media. *Journal of Electroanalytical Chemistry*, **2021**, 896, 115076	4.1	4
50	Coupling Surface Coverage and Electrostatic Effects on the Interfacial Adlayer–Water Structure of Hydrogenated Single-Crystal Platinum Electrodes. *Journal of Physical Chemistry C*, **2020**, 124, 13706-13714	3.8	10
49	Revisiting the Volmer-Heyrovský mechanism of hydrogen evolution on a nitrogen doped carbon nanotube: constrained molecular dynamics versus the nudged elastic band method. *Physical Chemistry Chemical Physics*, **2020**, 22, 10536-10549	3.6	21
48	Hydrogen Evolution Reaction on the Single-Shell Carbon-Encapsulated Iron Nanoparticle: A Density Functional Theory Insight. *Journal of Physical Chemistry C*, **2019**, 123, 13569-13577	3.8	10
47	Computational exploration of Fe55@C240-catalyzed Fischer-Tropsch synthesis. *Physical Chemistry Chemical Physics*, **2018**, 20, 2741-2753	3.6	2
46	Oxygen Evolution Reaction on Nitrogen-Doped Defective Carbon Nanotubes and Graphene. *Journal of Physical Chemistry C*, **2018**, 122, 25882-25892	3.8	46
45	Experimental and Computational Investigation of Hydrogen Evolution Reaction Mechanism on Nitrogen Functionalized Carbon Nanotubes. *ChemCatChem*, **2018**, 10, 3872-3882	5.2	11
44	FeNi Nanoparticles: A Multiscale First-Principles Study to Predict Geometry, Structure, and Catalytic Activity. *Journal of Physical Chemistry C*, **2017**, 121, 1667-1674	3.8	17
43	Electrochemical Activation of Single-Walled Carbon Nanotubes with Pseudo-Atomic-Scale Platinum for the Hydrogen Evolution Reaction. *ACS Catalysis*, **2017**, 7, 3121-3130	13.1	216
42	Functionalized Carbon Nanotubes with Ni(II) Bipyridine Complexes as Efficient Catalysts for the Alkaline Oxygen Evolution Reaction. *ACS Catalysis*, **2017**, 7, 8033-8041	13.1	46
41	Maghemite nanoparticles decorated on carbon nanotubes as efficient electrocatalysts for the oxygen evolution reaction. *Journal of Materials Chemistry A*, **2016**, 4, 5216-5222	13	55
40	Charge distribution and Fermi level in bimetallic nanoparticles. *Physical Chemistry Chemical Physics*, **2016**, 18, 2924-31	3.6	34
39	Ab Initio Electrochemistry: Exploring the Hydrogen Evolution Reaction on Carbon Nanotubes. *Journal of Physical Chemistry C*, **2015**, 119, 16166-16178	3.8	32
38	Theoretical Insight into the Hydrogen Evolution Activity of Open-Ended Carbon Nanotubes. *Journal of Physical Chemistry Letters*, **2015**, 6, 3956-60	6.4	25
37	Single-shell carbon-encapsulated iron nanoparticles: synthesis and high electrocatalytic activity for hydrogen evolution reaction. *Angewandte Chemie - International Edition*, **2015**, 54, 4535-8	16.4	238
36	The molecular and magnetic structure of carbon-enclosed and partially covered Fe55 particles. *Physical Chemistry Chemical Physics*, **2014**, 16, 3648-60	3.6	15
35	Competition between Icosahedral Motifs in AgCu, AgNi, and AgCo Nanoalloys: A Combined Atomistic–DFT Study. *Journal of Physical Chemistry C*, **2013**, 117, 26405-26413	3.8	110

34	Experimental and computational studies of nitrogen doped Degussa P25 TiO2: application to visible-light driven photo-oxidation of As(III). *Catalysis Science and Technology*, **2012**, 2, 784	5.5	32
33	Synthesis, structure, and complexation properties of hydroxybenzyl analogs of diethylenetriaminepentaacetic acid. *Journal of Coordination Chemistry*, **2010**, 63, 2026-2041	1.6	
32	Theoretical Study of the Hydrolysis of Pentameric Aluminum Complexes. *Journal of Chemical Theory and Computation*, **2010**, 6, 993-1007	6.4	17
31	Mechanism study of floating catalyst CVD synthesis of SWCNTs. *Physica Status Solidi (B): Basic Research*, **2010**, 247, 2708-2712	1.3	6
30	CO dissociation and CO+O reactions on a nanosized iron cluster. *Nano Research*, **2009**, 2, 660-670	10	36
29	CO Disproportionation on a Nanosized Iron Cluster. *Journal of Physical Chemistry C*, **2009**, 113, 12939-12942	3.8	13
28	Density functional studies of the hydrolysis of aluminum (chloro)hydroxide in water with CPMD and COSMO. *Journal of Physical Chemistry A*, **2008**, 112, 10873-80	2.8	17
27	A density functional study on water-sulfuric acid-ammonia clusters and implications for atmospheric cluster formation. *Journal of Geophysical Research*, **2007**, 112,		102
26	Ab initio molecular dynamics study of a mixture of HF(aq) and HCl(aq). *Journal of Physical Chemistry B*, **2006**, 110, 12699-706	3.4	8
25	Coadsorption of CO and O2 on Pd(1 1 1). *Chemical Physics*, **2005**, 314, 19-24	2.3	7
24	Partially and fully deprotonated sulfuric acid in H2SO4(H2O)n (n=6) clusters. *Chemical Physics Letters*, **2004**, 390, 307-313	2.5	35
23	Structure and dynamics of concentrated hydrochloric acid solutions. A first principles molecular dynamics study. *Physical Chemistry Chemical Physics*, **2004**, 6, 555-565	3.6	25
22	Nuclear magnetic shielding and quadrupole coupling tensors in liquid water: a combined molecular dynamics simulation and quantum chemical study. *Journal of the American Chemical Society*, **2004**, 126, 11093-102	16.4	57
21	Reliable potential for small sulfuric acid–water clusters. *Chemical Physics*, **2003**, 287, 7-19	2.3	35
20	Density functional complexation study of metal ions with (amino) polycarboxylic acid ligands. *Physical Chemistry Chemical Physics*, **2003**, 5, 3382-3393	3.6	37
19	Two Sulfuric Acids in Small Water Clusters. *Journal of Physical Chemistry A*, **2003**, 107, 8648-8658	2.8	68
18	Structural and Spectral Properties of Aqueous Hydrogen Fluoride Studied Using ab Initio Molecular Dynamics. *Journal of Physical Chemistry B*, **2002**, 106, 11315-11322	3.4	41
17	Coadsorption of CO and NO on the Pd(111) surface: combined ab initio and Monte Carlo study. *Physical Review Letters*, **2001**, 86, 5942-5	7.4	28

16	Ab initio study of O2 precursor states on the Pd(111) surface. *Journal of Chemical Physics*, **2001**, 115, 2297-2302	3.9	70
15	CO and NO adsorption and co-adsorption on the Pd(1 1 1) surface. *Surface Science*, **2001**, 489, 72-82	1.8	53
14	Oxygen molecule dissociation on the Al(111) surface. *Physical Review Letters*, **2000**, 84, 705-8	7.4	99
13	Ab initio study of gas-phase sulphuric acid hydrates containing 1 to 3 water molecules. *Journal of Chemical Physics*, **1998**, 108, 1031-1039	3.9	110
12	The torsional potential of perfluoro n-alkanes: A density functional study. *Journal of Chemical Physics*, **1996**, 104, 3692-3700	3.9	48
11	Ab initio molecular dynamics study of dilute hydrofluoric acid. *Molecular Physics*, **1996**, 88, 135-142	1.7	35
10	Ab Initio Molecular Dynamics Simulation of the Solvation and Transport of H3O+ and OH- Ions in Water. *The Journal of Physical Chemistry*, **1995**, 99, 5749-5752		493
9	Structure of CAl12. *Journal of Chemical Physics*, **1995**, 103, 8075-8080	3.9	25
8	Structural dynamics of protonated methane and acetylene. *Physical Review Letters*, **1995**, 74, 876-879	7.4	34
7	Ab Initio Molecular Dynamics Study of Hydrochloric Acid in Water. *Journal of the American Chemical Society*, **1994**, 116, 11620-11621	16.4	80
6	Car-Parrinello molecular dynamics with Vanderbilt ultrasoft pseudopotentials. *Physical Review B*, **1993**, 47, 10142-10153	3.3	1181
5	Ab initio molecular dynamics: application to liquid copper. *Computational Materials Science*, **1993**, 1, 419-427	3.3	
4	Ab initio studies on the structural and dynamical properties of ice. *Physical Review B*, **1993**, 47, 4863-4872	3.3	149
3	Ab initio studies on high pressure phases of ice. *Physical Review Letters*, **1992**, 69, 462-465	7.4	154
2	Ab initio molecular dynamics for d-electron systems: Liquid copper at 1500 K. *Physical Review Letters*, **1992**, 69, 1982-1985	7.4	333
1	Implementation of ultrasoft pseudopotentials in ab initio molecular dynamics. *Physical Review B*, **1991**, 43, 6796-6799	3.3	382