

# Kari Laasonen

## List of Publications by Citations

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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	Car-Parrinello molecular dynamics with Vanderbilt ultrasoft pseudopotentials. <i>Physical Review B</i> , <b>1993</b> , 47, 10142-10153	3.3	1181
50	Ab Initio Molecular Dynamics Simulation of the Solvation and Transport of H <sub>3</sub> O <sup>+</sup> and OH <sup>-</sup> Ions in Water. <i>The Journal of Physical Chemistry</i> , <b>1995</b> , 99, 5749-5752		493
49	Implementation of ultrasoft pseudopotentials in ab initio molecular dynamics. <i>Physical Review B</i> , <b>1991</b> , 43, 6796-6799	3.3	382
48	Ab initio molecular dynamics for d-electron systems: Liquid copper at 1500 K. <i>Physical Review Letters</i> , <b>1992</b> , 69, 1982-1985	7.4	333
47	Single-shell carbon-encapsulated iron nanoparticles: synthesis and high electrocatalytic activity for hydrogen evolution reaction. <i>Angewandte Chemie - International Edition</i> , <b>2015</b> , 54, 4535-8	16.4	238
46	Electrochemical Activation of Single-Walled Carbon Nanotubes with Pseudo-Atomic-Scale Platinum for the Hydrogen Evolution Reaction. <i>ACS Catalysis</i> , <b>2017</b> , 7, 3121-3130	13.1	216
45	Ab initio studies on high pressure phases of ice. <i>Physical Review Letters</i> , <b>1992</b> , 69, 462-465	7.4	154
44	Ab initio studies on the structural and dynamical properties of ice. <i>Physical Review B</i> , <b>1993</b> , 47, 4863-4873	3.3	149
43	Competition between Icosahedral Motifs in AgCu, AgNi, and AgCo Nanoalloys: A Combined Atomistic DFT Study. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 26405-26413	3.8	110
42	Ab initio study of gas-phase sulphuric acid hydrates containing 1 to 3 water molecules. <i>Journal of Chemical Physics</i> , <b>1998</b> , 108, 1031-1039	3.9	110
41	A density functional study on water-sulfuric acid-ammonia clusters and implications for atmospheric cluster formation. <i>Journal of Geophysical Research</i> , <b>2007</b> , 112,		102
40	Oxygen molecule dissociation on the Al(111) surface. <i>Physical Review Letters</i> , <b>2000</b> , 84, 705-8	7.4	99
39	Ab Initio Molecular Dynamics Study of Hydrochloric Acid in Water. <i>Journal of the American Chemical Society</i> , <b>1994</b> , 116, 11620-11621	16.4	80
38	Ab initio study of O <sub>2</sub> precursor states on the Pd(111) surface. <i>Journal of Chemical Physics</i> , <b>2001</b> , 115, 2297-2302	3.9	70
37	Two Sulfuric Acids in Small Water Clusters. <i>Journal of Physical Chemistry A</i> , <b>2003</b> , 107, 8648-8658	2.8	68
36	Nuclear magnetic shielding and quadrupole coupling tensors in liquid water: a combined molecular dynamics simulation and quantum chemical study. <i>Journal of the American Chemical Society</i> , <b>2004</b> , 126, 11093-102	16.4	57
35	Maghemite nanoparticles decorated on carbon nanotubes as efficient electrocatalysts for the oxygen evolution reaction. <i>Journal of Materials Chemistry A</i> , <b>2016</b> , 4, 5216-5222	13	55

34	CO and NO adsorption and co-adsorption on the Pd(1 1 1) surface. <i>Surface Science</i> , <b>2001</b> , 489, 72-82	1.8	53
33	The torsional potential of perfluoro n-alkanes: A density functional study. <i>Journal of Chemical Physics</i> , <b>1996</b> , 104, 3692-3700	3.9	48
32	Functionalized Carbon Nanotubes with Ni(II) Bipyridine Complexes as Efficient Catalysts for the Alkaline Oxygen Evolution Reaction. <i>ACS Catalysis</i> , <b>2017</b> , 7, 8033-8041	13.1	46
31	Oxygen Evolution Reaction on Nitrogen-Doped Defective Carbon Nanotubes and Graphene. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 25882-25892	3.8	46
30	Structural and Spectral Properties of Aqueous Hydrogen Fluoride Studied Using ab Initio Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , <b>2002</b> , 106, 11315-11322	3.4	41
29	Density Functional complexation study of metal ions with (amino) polycarboxylic acid ligands. <i>Physical Chemistry Chemical Physics</i> , <b>2003</b> , 5, 3382-3393	3.6	37
28	CO dissociation and CO+O reactions on a nanosized iron cluster. <i>Nano Research</i> , <b>2009</b> , 2, 660-670	10	36
27	Partially and fully deprotonated sulfuric acid in H <sub>2</sub> SO <sub>4</sub> (H <sub>2</sub> O) <sub>n</sub> (n=69) clusters. <i>Chemical Physics Letters</i> , <b>2004</b> , 390, 307-313	2.5	35
26	Reliable potential for small sulfuric acid/water clusters. <i>Chemical Physics</i> , <b>2003</b> , 287, 7-19	2.3	35
25	Ab initio molecular dynamics study of dilute hydrofluoric acid. <i>Molecular Physics</i> , <b>1996</b> , 88, 135-142	1.7	35
24	Charge distribution and Fermi level in bimetallic nanoparticles. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 2924-31	3.6	34
23	Structural dynamics of protonated methane and acetylene. <i>Physical Review Letters</i> , <b>1995</b> , 74, 876-879	7.4	34
22	Ab Initio Electrochemistry: Exploring the Hydrogen Evolution Reaction on Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 16166-16178	3.8	32
21	Experimental and computational studies of nitrogen doped Degussa P25 TiO <sub>2</sub> : application to visible-light driven photo-oxidation of As(III). <i>Catalysis Science and Technology</i> , <b>2012</b> , 2, 784	5.5	32
20	Coadsorption of CO and NO on the Pd(111) surface: combined ab initio and Monte Carlo study. <i>Physical Review Letters</i> , <b>2001</b> , 86, 5942-5	7.4	28
19	Theoretical Insight into the Hydrogen Evolution Activity of Open-Ended Carbon Nanotubes. <i>Journal of Physical Chemistry Letters</i> , <b>2015</b> , 6, 3956-60	6.4	25
18	Structure and dynamics of concentrated hydrochloric acid solutions. A first principles molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , <b>2004</b> , 6, 555-565	3.6	25
17	Structure of CA12. <i>Journal of Chemical Physics</i> , <b>1995</b> , 103, 8075-8080	3.9	25

16	Revisiting the Volmer-Heyrovskĳmechanism of hydrogen evolution on a nitrogen doped carbon nanotube: constrained molecular dynamics versus the nudged elastic band method. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 10536-10549	3.6	21
15	FeNi Nanoparticles: A Multiscale First-Principles Study to Predict Geometry, Structure, and Catalytic Activity. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 1667-1674	3.8	17
14	Theoretical Study of the Hydrolysis of Pentameric Aluminum Complexes. <i>Journal of Chemical Theory and Computation</i> , <b>2010</b> , 6, 993-1007	6.4	17
13	Density functional studies of the hydrolysis of aluminum (chloro)hydroxide in water with CPMD and COSMO. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 10873-80	2.8	17
12	The molecular and magnetic structure of carbon-enclosed and partially covered Fe <sub>55</sub> particles. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 3648-60	3.6	15
11	CO Disproportionation on a Nanosized Iron Cluster. <i>Journal of Physical Chemistry C</i> , <b>2009</b> , 113, 12939-12942	3.4	13
10	Experimental and Computational Investigation of Hydrogen Evolution Reaction Mechanism on Nitrogen Functionalized Carbon Nanotubes. <i>ChemCatChem</i> , <b>2018</b> , 10, 3872-3882	5.2	11
9	Hydrogen Evolution Reaction on the Single-Shell Carbon-Encapsulated Iron Nanoparticle: A Density Functional Theory Insight. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 13569-13577	3.8	10
8	Coupling Surface Coverage and Electrostatic Effects on the Interfacial Adlayer/Water Structure of Hydrogenated Single-Crystal Platinum Electrodes. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 13706-13714	3.8	10
7	Ab initio molecular dynamics study of a mixture of HF(aq) and HCl(aq). <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 12699-706	3.4	8
6	Coadsorption of CO and O <sub>2</sub> on Pd(1 1 1). <i>Chemical Physics</i> , <b>2005</b> , 314, 19-24	2.3	7
5	Mechanism study of floating catalyst CVD synthesis of SWCNTs. <i>Physica Status Solidi (B): Basic Research</i> , <b>2010</b> , 247, 2708-2712	1.3	6
4	Designing of low Pt electrocatalyst through immobilization on metal@C support for efficient hydrogen evolution reaction in acidic media. <i>Journal of Electroanalytical Chemistry</i> , <b>2021</b> , 896, 115076	4.1	4
3	Computational exploration of Fe <sub>55</sub> @C <sub>240</sub> -catalyzed Fischer-Tropsch synthesis. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 2741-2753	3.6	2
2	Synthesis, structure, and complexation properties of hydroxybenzyl analogs of diethylenetriaminepentaacetic acid. <i>Journal of Coordination Chemistry</i> , <b>2010</b> , 63, 2026-2041	1.6	
1	Ab initio molecular dynamics: application to liquid copper. <i>Computational Materials Science</i> , <b>1993</b> , 1, 419-427		