Ali Kachmar

List of Publications by Year
in descending order

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25 papers	566 citations	858243 12 h-index	685536 24 g-index
27 all docs	27 docs citations	27 times ranked	1238 citing authors

#	Article	IF	Citations
1	Iodide vs Chloride: The Impact of Different Lead Halides on the Solution Chemistry of Perovskite Precursors. ACS Applied Energy Materials, 2021, 4, 9827-9835.	2.5	11
2	First-Principles Molecular Dynamics in Metal-Halide Perovskites: Contrasting Generalized Gradient Approximation and Hybrid Functionals. Journal of Physical Chemistry Letters, 2021, 12, 11886-11893.	2.1	13
3	Structural and Optical Properties of Solvated PbI₂ in Î³-Butyrolactone: Insight into the Solution Chemistry of Lead Halide Perovskite Precursors. Journal of Physical Chemistry Letters, 2020, 11, 6139-6145.	2.1	15
4	Crystallization properties of arsenic doped GST alloys. Scientific Reports, 2019, 9, 12985.	1.6	14
5	Effect of Water on the Structural, Optical, and Hot-Carrier Cooling Properties of the Perovskite Material MASnI₃. Journal of Physical Chemistry C, 2019, 123, 4056-4063.	1.5	13
6	Role of Water on the Rotational Dynamics of the Organic Methylammonium Cation: A First Principles Analysis. Scientific Reports, 2019, 9, 668.	1.6	15
7	Effects of Electronâ€“Phonon Coupling on Electronic Properties of Methylammonium Lead Iodide Perovskites. Journal of Physical Chemistry Letters, 2018, 9, 7090-7097.	2.1	44
8	New insights into the atomic structure of amorphous TiO2 using tight-binding molecular dynamics. Journal of Chemical Physics, 2018, 149, 094501.	1.2	11
9	Free Energy Landscape of Sodium Solvation into Graphite. Journal of Physical Chemistry C, 2018, 122, 20064-20072.	1.5	9
10	Mapping the Free Energy of Lithium Solvation in the Protic Ionic Liquid Ethylammonuim Nitrate: A Metadynamics Study. ChemSusChem, 2017, 10, 3083-3090.	3.6	10
11	First-Principles Study of the Transport Properties in Bulk and Monolayer MX₃ (M = Ti, Zr,) Tj ETQq1 1 0.784314 rgBT /Ov	1.5	34
12	Role of Cations on the Electronic Transport and Optical Properties of Lead-Iodide Perovskites. Journal of Physical Chemistry C, 2016, 120, 16259-16270.	1.5	56
13	Thermal Effects on CH₃NH₃PbI₃ Perovskite from Ab Initio Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2015, 119, 8991-8997.	1.5	112
14	Structural, dynamic, electronic, and vibrational properties of flexible, intermediate, and stressed rigid As-Se glasses and liquids from first principles molecular dynamics. Journal of Chemical Physics, 2014, 141, 194506.	1.2	37
15	An efficient and cyclic hydrogen evolution reaction mechanism on [Ni(PH2NH2)2]2+ catalysts: a theoretical and multiscale simulation study. RSC Advances, 2014, 4, 5177.	1.7	4
16	Tetrahedral germanium in amorphous phase change materials: Exploring the isochemical scenario. Physica Status Solidi (B): Basic Research, 2012, 249, 1890-1896.	0.7	9
17	New Insights in the Electrocatalytic Proton Reduction and Hydrogen Oxidation by Bioinspired Catalysts: A DFT Investigation. Journal of Physical Chemistry A, 2010, 114, 11861-11867.	1.1	17
18	Multi-scale Modeling-based Prediction of PEM Fuel Cells MEA Durability under Automotive Operating Conditions. ECS Transactions, 2009, 25, 65-79.	0.3	13

#	Article	IF	Citations
19	Conformational Changes in a Flexible, Encapsulated Dicarboxylate: Evidence from Density Functional Theory Simulations. Journal of Physical Chemistry A, 2009, 113, 9075-9079.	1.1	4
20	Dynamic Properties of a Hexadecamolybdenum Wheel: Studies in Solution and Density Functional Theory Calculations. Inorganic Chemistry, 2009, 48, 6852-6859.	1.9	9
21	The â€œhydrazinoturnâ€•hydrogen bonding network in hydrazinopeptides and aza-Î²3-peptides as probed by an AIM topological analysis of the electronic density. Computational and Theoretical Chemistry, 2008, 869, 41-46.	1.5	8
22	Tuning the thermodynamic stability of oxothiomolybdenum wheels: crystal structures, studies in solution and DFT calculations. Dalton Transactions, 2008, , 4565.	1.6	23
23	A New Class of Efficient Electrocatalysts for the Reduction of Protons into Hydrogen Based on the [Mo₂O₂S₂]²⁺ Building Block. Journal of Physical Chemistry C, 2008, 112, 1109-1114.	1.5	42
24	Hostâ€“guest adaptability within oxothiomolybdenum wheels: structures, studies in solution and DFT calculations. Dalton Transactions, 2007, , 3043-3054.	1.6	37
25	Changing the Oxothiomolybdate Ring from an Anionic to a Cationic Receptor. Inorganic Chemistry, 2007, 46, 9516-9518.	1.9	6