

MikaÃ«l Kepenekian

List of Publications by Year in descending order

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67
papers

5,825
citations

182225

30
h-index

124990

64
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68
all docs

68
docs citations

68
times ranked

7378
citing authors

#	ARTICLE	IF	CITATIONS
1	Band gap, effective masses, and energy level alignment of 2D and 3D halide perovskites and heterostructures using DFT-1/2. <i>Physical Review Materials</i> , 2022, 6, .	0.9	13
2	Tolerance Factor for Stabilizing 3D Hybrid Halide Perovskitoids Using Linear Diammonium Cations. <i>Journal of the American Chemical Society</i> , 2022, 144, 3902-3912.	6.6	36
3	Thick-Layer Lead Iodide Perovskites with Bifunctional Organic Spacers Allylammonium and Iodopropylammonium Exhibiting Trap-State Emission. <i>Journal of the American Chemical Society</i> , 2022, 144, 6390-6409.	6.6	13
4	Pb-free halide perovskites for solar cells, light-emitting diodes, and photocatalysts. <i>APL Materials</i> , 2022, 10, .	2.2	11
5	Interplay between Electronic, Magnetic, and Transport Properties in Metal Organic Radical Frameworks. <i>Journal of Physical Chemistry C</i> , 2021, 125, 11225-11234.	1.5	3
6	Shedding Light on the Stability and Structure-Property Relationships of Two-Dimensional Hybrid Lead Bromide Perovskites. <i>Chemistry of Materials</i> , 2021, 33, 5085-5107.	3.2	29
7	Bismuth/Silver-Based Two-Dimensional Iodide Double and One-Dimensional Bi Perovskites: Interplay between Structural and Electronic Dimensions. <i>Chemistry of Materials</i> , 2021, 33, 6206-6216.	3.2	27
8	From Zero- to One-Dimensional, Opportunities and Caveats of Hybrid Iodobismuthates for Optoelectronic Applications. <i>Inorganic Chemistry</i> , 2021, 60, 17123-17131.	1.9	13
9	Electronic structure and stability of Cs ₂ TiX ₆ and Cs ₂ ZrX ₆ (X = Br, I) vacancy ordered double perovskites. <i>Applied Physics Letters</i> , 2021, 119, .	1.5	28
10	A 3D Lead Iodide Hybrid Based on a 2D Perovskite Subnetwork. <i>Crystals</i> , 2021, 11, 1570.	1.0	2
11	Importance of Vacancies and Doping in the Hole-Transporting Nickel Oxide Interface with Halide Perovskites. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 6633-6640.	4.0	21
12	Three-Dimensional Lead Iodide Perovskitoid Hybrids with High X-ray Photoresponse. <i>Journal of the American Chemical Society</i> , 2020, 142, 6625-6637.	6.6	82
13	Negative Thermal Quenching in FASn ₃ Perovskite Single Crystals and Thin Films. <i>ACS Energy Letters</i> , 2020, 5, 2512-2519.	8.8	55
14	Water-Stable 1D Hybrid Tin(II) Iodide Emits Broad Light with 36% Photoluminescence Quantum Efficiency. <i>Journal of the American Chemical Society</i> , 2020, 142, 9028-9038.	6.6	57
15	Organic Cation Alloying on Intralayer A and Interlayer A sites in 2D Hybrid Dion-Jacobson Lead Bromide Perovskites (A)(Pb ₂ Br ₇). <i>Journal of the American Chemical Society</i> , 2020, 142, 8342-8351.	6.6	64
16	Two-Dimensional Dion-Jacobson Hybrid Lead Iodide Perovskites with Aromatic Diammonium Cations. <i>Journal of the American Chemical Society</i> , 2019, 141, 12880-12890.	6.6	241
17	Phase-Transition-Induced Carrier Mass Enhancement in 2D Ruddlesden-Popper Perovskites. <i>ACS Energy Letters</i> , 2019, 4, 2386-2392.	8.8	38
18	Efficient and accurate calculation of band gaps of halide perovskites with the Tran-Blaha modified Becke-Johnson potential. <i>Physical Review B</i> , 2019, 99, .	1.1	61

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19	Red-NIR luminescence of Mo ₆ monolayered assembly directly anchored on Au(001). <i>Materials Horizons</i> , 2019, 6, 1828-1833.	6.4	12
20	From 2D to 1D Electronic Dimensionality in Halide Perovskites with Stepped and Flat Layers Using Propylammonium as a Spacer. <i>Journal of the American Chemical Society</i> , 2019, 141, 10661-10676.	6.6	66
21	Charge Trap Formation and Passivation in Methylammonium Lead Tribromide. <i>Journal of Physical Chemistry C</i> , 2019, 123, 13812-13817.	1.5	9
22	Enhanced Stability and Band Gap Tuning of $\text{[HC(NH}_2\text{)]}_2\text{PbI}_3$ Hybrid Perovskite by Large Cation Integration. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 20743-20751.	4.0	52
23	Small Cyclic Diammonium Cation Templated (110)-Oriented 2D Halide (X = I, Br, Cl) Perovskites with White-Light Emission. <i>Chemistry of Materials</i> , 2019, 31, 3582-3590.	3.2	101
24	Guanidinium and Mixed Cesium-Guanidinium Tin(II) Bromides: Effects of Quantum Confinement and Out-of-Plane Octahedral Tilting. <i>Chemistry of Materials</i> , 2019, 31, 2121-2129.	3.2	24
25	Electronic properties of Pb-I deficient lead halide perovskites. <i>Journal of Chemical Physics</i> , 2019, 151, 234704.	1.2	7
26	Structural and thermodynamic limits of layer thickness in 2D halide perovskites. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 58-66.	3.3	236
27	Composite Nature of Layered Hybrid Perovskites: Assessment on Quantum and Dielectric Confinements and Band Alignment. <i>ACS Nano</i> , 2018, 12, 3321-3332.	7.3	146
28	Does Rashba splitting in $\text{CH}_3\text{NH}_3\text{PbBr}_3$ arise from 2 Å ⁻² surface reconstruction?. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 9638-9643.	1.3	29
29	Structural Diversity in White-Light-Emitting Hybrid Lead Bromide Perovskites. <i>Journal of the American Chemical Society</i> , 2018, 140, 13078-13088.	6.6	351
30	Two-Dimensional Halide Perovskites Incorporating Straight Chain Symmetric Diammonium Ions, $(\text{NH}_3\text{C}_m\text{H}_{2m}\text{NH}_3)(\text{CH}_3\text{NH}_3)_2\text{PbI}_3$ ($m = 4, 9; n = 1, 4$). <i>Journal of the American Chemical Society</i> , 2018, 140, 12226-12238.	6.6	374
31	Concept of Lattice Mismatch and Emergence of Surface States in Two-dimensional Hybrid Perovskite Quantum Wells. <i>Nano Letters</i> , 2018, 18, 5603-5609.	4.5	103
32	Scaling law for excitons in 2D perovskite quantum wells. <i>Nature Communications</i> , 2018, 9, 2254.	5.8	559
33	Extremely efficient internal exciton dissociation through edge states in layered 2D perovskites. <i>Science</i> , 2017, 355, 1288-1292.	6.0	830
34	New Type of 2D Perovskites with Alternating Cations in the Interlayer Space, $(\text{C}(\text{NH}_2)_3)_3(\text{CH}_3\text{NH}_3)_3\text{PbI}_3$ Structure, Properties, and Photovoltaic Performance. <i>Journal of the American Chemical Society</i> , 2017, 139, 16297-16309.	6.6	374
35	Enhanced Cooperativity in Supported Spin-Crossover Metal-Organic Frameworks. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 3415-3420.	2.1	17
36	Rashba and Dresselhaus Couplings in Halide Perovskites: Accomplishments and Opportunities for Spintronics and Spin-Orbitronics. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 3362-3370.	2.1	150

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37	Decreasing the electronic confinement in layered perovskites through intercalation. <i>Chemical Science</i> , 2017, 8, 1960-1968.	3.7	114
38	Advances and Promises of Layered Halide Hybrid Perovskite Semiconductors. <i>ACS Nano</i> , 2016, 10, 9776-9786.	7.3	351
39	Thermal and near-infrared light induced spin crossover in a mononuclear iron(<i>ii</i>) complex with a tetrathiafulvalene-fused dipyridophenazine ligand. <i>Dalton Transactions</i> , 2016, 45, 11267-11271.	1.6	25
40	Quantum confinement and dielectric profiles of colloidal nanoplatelets of halide inorganic and hybrid organic-inorganic perovskites. <i>Nanoscale</i> , 2016, 8, 6369-6378.	2.8	136
41	Dielectric properties of hybrid perovskites and drift-diffusion modeling of perovskite cells. <i>Proceedings of SPIE</i> , 2016, , .	0.8	8
42	Theoretical studies of Rashba and Dresselhaus effects in hybrid organic-inorganic perovskites for optoelectronic applications. , 2016, , .		2
43	Interplay of spin-orbit coupling and lattice distortion in metal substituted 3D tri-chloride hybrid perovskites. <i>Journal of Materials Chemistry A</i> , 2015, 3, 9232-9240.	5.2	101
44	Solid-State Physics Perspective on Hybrid Perovskite Semiconductors. <i>Journal of Physical Chemistry C</i> , 2015, 119, 10161-10177.	1.5	205
45	Theoretical insights into multibandgap hybrid perovskites for photovoltaic applications. , 2015, , .		0
46	Rashba and Dresselhaus Effects in Hybrid Organic-Inorganic Perovskites: From Basics to Devices. <i>ACS Nano</i> , 2015, 9, 11557-11567.	7.3	304
47	Spin transport in dangling-bond wires on doped H-passivated Si(100). <i>Nanotechnology</i> , 2014, 25, 465703.	1.3	10
48	Electronic surface states and dielectric self-energy profiles in colloidal nanoscale platelets of CdSe. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 25182-25190.	1.3	30
49	Difficulties in theab initio description of electron transport through spin filters. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 104203.	0.7	6
50	Electron transport through dangling-bond silicon wires on H-passivated Si(100). <i>Journal of Physics Condensed Matter</i> , 2013, 25, 025503.	0.7	11
51	Surface-State Engineering for Interconnects on H-Passivated Si(100). <i>Nano Letters</i> , 2013, 13, 1192-1195.	4.5	31
52	Vibrational transition rule during a through-bond electron transfer process. <i>Chemical Physics Letters</i> , 2013, 567, 1-5.	1.2	5
53	Leakage current in atomic-size surface interconnects. <i>Applied Physics Letters</i> , 2013, 103, , .	1.5	4
54	First-Principles Simulations of Electronic Transport in Dangling-Bond Wires. <i>Advances in Atom and Single Molecule Machines</i> , 2013, , 137-147.	0.0	0

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55	A bottom-up valence bond derivation of excitation energies in 1D-like delocalized systems. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 1381-1388.	1.3	4
56	Crystal Structure, Spin Polarization, Solid-State Electrochemistry, and High n-Type Carrier Mobility of a Paramagnetic Semiconductor: Vanadyl Tetrakis(thiadiazole)porphyrazine. <i>Inorganic Chemistry</i> , 2012, 51, 456-462.	1.9	32
57	Energetics and stability of dangling-bond silicon wires on H passivated Si(100). <i>Journal of Physics Condensed Matter</i> , 2012, 24, 445004.	0.7	20
58	Magnetic and conduction properties in 1D organic radical materials: an ab initio inspection for a challenging quest. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 6657.	1.3	29
59	Toward Reliable DFT Investigations of Mn-Porphyrins through CASPT2/DFT Comparison. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3532-3539.	2.3	25
60	A New Route towards Redox Bistability through the Inspection of Manganese ^{II} -Porphyrin Complexes. <i>Chemistry - A European Journal</i> , 2011, 17, 12045-12050.	1.7	10
61	Suppression of the Peierls instability in 1D system: Semi-local approach to Little's conjecture. <i>Chemical Physics Letters</i> , 2010, 486, 40-43.	1.2	1
62	Reliability and Storage Capacity: a Compromise Illustrated in the Two-Step Spin-Crossover System [Fe(bapbp)(NCS) ₂]. <i>Inorganic Chemistry</i> , 2010, 49, 11057-11061.	1.9	26
63	Magnetic bistability: From microscopic to macroscopic understandings of hysteretic behavior using ab initio calculations. <i>Physical Review B</i> , 2009, 79, .	1.1	52
64	Energetics of [Fe(NCH) ₆] ²⁺ via CASPT2 calculations: A spin-crossover perspective. <i>Journal of Computational Chemistry</i> , 2009, 30, 2327-2333.	1.5	61
65	What zeroth-order Hamiltonian for CASPT2 adiabatic energetics of Fe(II)N ₆ architectures?. <i>Journal of Chemical Physics</i> , 2009, 131, 114702.	1.2	72
66	Ligands bonded to metal ion or through-metal interacting ligands? Analysis of unusual bonds formation in the (BDTA) ₂ [Co(mnt) ₂] material. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 6066.	1.3	16
67	Primary Role of the Electrostatic Contributions in a Rational Growth of Hysteresis Loop in Spin-Crossover Fe(II) Complexes. <i>Journal of the American Chemical Society</i> , 2009, 131, 11498-11502.	6.6	90