MikaÃ«l Kepenekian

List of Publications by Year
in descending order

67 papers	5,825 citations	159585 30 h-index	110387 64 g-index
68 all docs	68 docs citations	68 times ranked	6374 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. Physical Review Materials, 2022, 6, .	2.4	13
2	Tolerance Factor for Stabilizing 3D Hybrid Halide Perovskitoids Using Linear Diammonium Cations. Journal of the American Chemical Society, 2022, 144, 3902-3912.	13.7	36
3	Thick-Layer Lead Iodide Perovskites with Bifunctional Organic Spacers Allylammonium and Iodopropylammonium Exhibiting Trap-State Emission. Journal of the American Chemical Society, 2022, 144, 6390-6409.	13.7	13
4	Pb-free halide perovskites for solar cells, light-emitting diodes, and photocatalysts. APL Materials, 2022, 10, .	5.1	11
5	Interplay between Electronic, Magnetic, and Transport Properties in Metal Organicâ€“Radical Frameworks. Journal of Physical Chemistry C, 2021, 125, 11225-11234.	3.1	3
6	Shedding Light on the Stability and Structureâ€“Property Relationships of Two-Dimensional Hybrid Lead Bromide Perovskites. Chemistry of Materials, 2021, 33, 5085-5107.	6.7	29
7	Bismuth/Silver-Based Two-Dimensional Iodide Double and One-Dimensional Bi Perovskites: Interplay between Structural and Electronic Dimensions. Chemistry of Materials, 2021, 33, 6206-6216.	6.7	27
8	From Zero- to One-Dimensional, Opportunities and Caveats of Hybrid Iodobismuthates for Optoelectronic Applications. Inorganic Chemistry, 2021, 60, 17123-17131.	4.0	13
9	Electronic structure and stability of Cs2TiX6 and Cs2ZrX6 (X = Br, I) vacancy ordered double perovskites. Applied Physics Letters, 2021, 119, .	3.3	28
10	A 3D Lead Iodide Hybrid Based on a 2D Perovskite Subnetwork. Crystals, 2021, 11, 1570.	2.2	2
11	Importance of Vacancies and Doping in the Hole-Transporting Nickel Oxide Interface with Halide Perovskites. ACS Applied Materials & Interfaces, 2020, 12, 6633-6640.	8.0	21
12	Three-Dimensional Lead Iodide Perovskitoid Hybrids with High X-ray Photoresponse. Journal of the American Chemical Society, 2020, 142, 6625-6637.	13.7	82
13	Negative Thermal Quenching in FASnI₃ Perovskite Single Crystals and Thin Films. ACS Energy Letters, 2020, 5, 2512-2519.	17.4	55
14	Water-Stable 1D Hybrid Tin(II) Iodide Emits Broad Light with 36% Photoluminescence Quantum Efficiency. Journal of the American Chemical Society, 2020, 142, 9028-9038.	13.7	57
15	Organic Cation Alloying on Intralayer A and Interlayer Aâ€™ sites in 2D Hybrid Dionâ€“Jacobson Lead Bromide Perovskites (Aâ€™)(A)Pb₂Br₇. Journal of the American Chemical Society, 2020, 142, 8342-8351.	13.7	64
16	Two-Dimensional Dionâ€“Jacobson Hybrid Lead Iodide Perovskites with Aromatic Diammonium Cations. Journal of the American Chemical Society, 2019, 141, 12880-12890.	13.7	241
17	Phase-Transition-Induced Carrier Mass Enhancement in 2D Ruddlesdenâ€“Popper Perovskites. ACS Energy Letters, 2019, 4, 2386-2392.	17.4	38
18	Efficient and accurate calculation of band gaps of halide perovskites with the Tran-Blaha modified Becke-Johnson potential. Physical Review B, 2019, 99, .	3.2	61

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19	Red-NIR luminescence of Mo₆ monolayered assembly directly anchored on Au(001). Materials Horizons, 2019, 6, 1828-1833.	12.2	12
20	From 2D to 1D Electronic Dimensionality in Halide Perovskites with Stepped and Flat Layers Using Propylammonium as a Spacer. Journal of the American Chemical Society, 2019, 141, 10661-10676.	13.7	66
21	Charge Trap Formation and Passivation in Methylammonium Lead Tribromide. Journal of Physical Chemistry C, 2019, 123, 13812-13817.	3.1	9
22	Enhanced Stability and Band Gap Tuning of Î±-[HC(NH₂)₂]PbI₃ Hybrid Perovskite by Large Cation Integration. ACS Applied Materials & Interfaces, 2019, 11, 20743-20751.	8.0	52
23	Small Cyclic Diammonium Cation Templated (110)-Oriented 2D Halide (X = I, Br, Cl) Perovskites with White-Light Emission. Chemistry of Materials, 2019, 31, 3582-3590.	6.7	101
24	Guanidinium and Mixed Cesiumâ€“Guanidinium Tin(II) Bromides: Effects of Quantum Confinement and Out-of-Plane Octahedral Tilting. Chemistry of Materials, 2019, 31, 2121-2129.	6.7	24
25	Electronic properties of Pb-I deficient lead halide perovskites. Journal of Chemical Physics, 2019, 151, 234704.	3.0	7
26	Structural and thermodynamic limits of layer thickness in 2D halide perovskites. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 58-66.	7.1	236
27	Composite Nature of Layered Hybrid Perovskites: Assessment on Quantum and Dielectric Confinements and Band Alignment. ACS Nano, 2018, 12, 3321-3332.	14.6	146
28	Does Rashba splitting in CH₃NH₃PbBr₃ arise from 2 Ã— 2 surface reconstruction?. Physical Chemistry Chemical Physics, 2018, 20, 9638-9643.	2.8	29
29	Structural Diversity in White-Light-Emitting Hybrid Lead Bromide Perovskites. Journal of the American Chemical Society, 2018, 140, 13078-13088.	13.7	351
30	Two-Dimensional Halide Perovskites Incorporating Straight Chain Symmetric Diammonium Ions, (NH₃C_mH_{2m}NH₃)(CH₃NH₃)_nPb_nI_{3n+1} (m = 4â€“9; n = 1â€“4). Journal of the American Chemical Society, 2018, 140, 12226-12238.	13.7	184
31	Concept of Lattice Mismatch and Emergence of Surface States in Two-dimensional Hybrid Perovskite Quantum Wells. Nano Letters, 2018, 18, 5603-5609.	9.1	103
32	Scaling law for excitons in 2D perovskite quantum wells. Nature Communications, 2018, 9, 2254.	12.8	559
33	Extremely efficient internal exciton dissociation through edge states in layered 2D perovskites. Science, 2017, 355, 1288-1292.	12.6	830
34	New Type of 2D Perovskites with Alternating Cations in the Interlayer Space, (C(NH₂)₃)(CH₃NH₃)_nPb_nI_{3n} Structure, Properties, and Photovoltaic Performance. Journal of the American Chemical Society, 2017, 139, 16297-16309.	13.7	374
35	Enhanced Cooperativity in Supported Spin-Crossover Metalâ€“Organic Frameworks. Journal of Physical Chemistry Letters, 2017, 8, 3415-3420.	4.6	17
36	Rashba and Dresselhaus Couplings in Halide Perovskites: Accomplishments and Opportunities for Spintronics and Spinâ€“Orbitronics. Journal of Physical Chemistry Letters, 2017, 8, 3362-3370.	4.6	150

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37	Decreasing the electronic confinement in layered perovskites through intercalation. Chemical Science, 2017, 8, 1960-1968.	7.4	114
38	Advances and Promises of Layered Halide Hybrid Perovskite Semiconductors. ACS Nano, 2016, 10, 9776-9786.	14.6	351
39	Thermal and near-infrared light induced spin crossover in a mononuclear iron(<scp>ii</scp>) complex with a tetrathiafulvalene-fused dipyridophenazine ligand. Dalton Transactions, 2016, 45, 11267-11271.	3.3	25
40	Quantum confinement and dielectric profiles of colloidal nanoplatelets of halide inorganic and hybrid organicâ€“inorganic perovskites. Nanoscale, 2016, 8, 6369-6378.	5.6	136
41	Dielectric properties of hybrid perovskites and drift-diffusion modeling of perovskite cells. Proceedings of SPIE, 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 spinâ€“orbit coupling and lattice distortion in metal substituted 3D tri-chloride hybrid perovskites. Journal of Materials Chemistry A, 2015, 3, 9232-9240.	10.3	101
44	Solid-State Physics Perspective on Hybrid Perovskite Semiconductors. Journal of Physical Chemistry C, 2015, 119, 10161-10177.	3.1	205
45	Theoretical insights into multibandgap hybrid perovskites for photovoltaic applications. , 2015, , .		0
46	Rashba and Dresselhaus Effects in Hybrid Organicâ€“Inorganic Perovskites: From Basics to Devices. ACS Nano, 2015, 9, 11557-11567.	14.6	304
47	Spin transport in dangling-bond wires on doped H-passivated Si(100). Nanotechnology, 2014, 25, 465703.	2.6	10
48	Electronic surface states and dielectric self-energy profiles in colloidal nanoscale platelets of CdSe. Physical Chemistry Chemical Physics, 2014, 16, 25182-25190.	2.8	30
49	Difficulties in theab initiodescription of electron transport through spin filters. Journal of Physics Condensed Matter, 2014, 26, 104203.	1.8	6
50	Electron transport through dangling-bond silicon wires on H-passivated Si(100). Journal of Physics Condensed Matter, 2013, 25, 025503.	1.8	11
51	Surface-State Engineering for Interconnects on H-Passivated Si(100). Nano Letters, 2013, 13, 1192-1195.	9.1	31
52	Vibrational transition rule during a through-bond electron transfer process. Chemical Physics Letters, 2013, 567, 1-5.	2.6	5
53	Leakage current in atomic-size surface interconnects. Applied Physics Letters, 2013, 103, .	3.3	4
54	First-Principles Simulations of Electronic Transport in Dangling-Bond Wires. Advances in Atom and Single Molecule Machines, 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. Physical Chemistry Chemical Physics, 2012, 14, 1381-1388.	2.8	4
56	Crystal Structure, Spin Polarization, Solid-State Electrochemistry, and High n-Type Carrier Mobility of a Paramagnetic Semiconductor: Vanadyl Tetrakis(thiadiazole)porphyrazine. Inorganic Chemistry, 2012, 51, 456-462.	4.0	32
57	Energetics and stability of dangling-bond silicon wires on H passivated Si(100). Journal of Physics Condensed Matter, 2012, 24, 445004.	1.8	20
58	Magnetic and conduction properties in 1D organic radical materials: an ab initio inspection for a challenging quest. Physical Chemistry Chemical Physics, 2011, 13, 6657.	2.8	29
59	Toward Reliable DFT Investigations of Mn-Porphyrins through CASPT2/DFT Comparison. Journal of Chemical Theory and Computation, 2011, 7, 3532-3539.	5.3	25
60	A New Route towards Redox Bistability through the Inspection of Manganeseâ€“Porphyrin Complexes. Chemistry - A European Journal, 2011, 17, 12045-12050.	3.3	10
61	Suppression of the Peierls instability in 1D system: Semi-local approach to Littleâ€™s conjecture. Chemical Physics Letters, 2010, 486, 40-43.	2.6	1
62	Reliability and Storage Capacity: a Compromise Illustrated in the Two-Step Spin-Crossover System [Fe(bapbpy)(NCS)₂]. Inorganic Chemistry, 2010, 49, 11057-11061.	4.0	26
63	Magnetic bistability: From microscopic to macroscopic understandings of hysteretic behavior usingab initiocalculations. Physical Review B, 2009, 79, .	3.2	52
64	Energetics of [Fe(NCH)₆]²⁺ via CASPT2 calculations: A spinâ€crossover perspective. Journal of Computational Chemistry, 2009, 30, 2327-2333.	3.3	61
65	What zeroth-order Hamiltonian for CASPT2 adiabatic energetics of Fe(II)N6 architectures?. Journal of Chemical Physics, 2009, 131, 114702.	3.0	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. Physical Chemistry Chemical Physics, 2009, 11, 6066.	2.8	16
67	Primary Role of the Electrostatic Contributions in a Rational Growth of Hysteresis Loop in Spin-Crossover Fe(II) Complexes. Journal of the American Chemical Society, 2009, 131, 11498-11502.	13.7	90