Maria K Y Chan

List of Publications by Year
in descending order

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104 papers	7,418 citations	126907 33 h-index	53230 85 g-index
106 all docs	106 docs citations	106 times ranked	12742 citing authors

#	Article	IF	Citations
1	Trends in activity for the water electrolyser reactions on 3d M(Ni,Co,Fe,Mn) hydr(oxy)oxide catalysts. Nature Materials, 2012, 11, 550-557.	27.5	2,423
2	Ultralow-loading platinum-cobalt fuel cell catalysts derived from imidazolate frameworks. Science, 2018, 362, 1276-1281.	12.6	735
3	Edge-terminated molybdenum disulfide with a 9.4-Ã... interlayer spacing for electrochemical hydrogen production. Nature Communications, 2015, 6, 7493.	12.8	628
4	Efficient Band Gap Prediction for Solids. Physical Review Letters, 2010, 105, 196403.	7.8	398
5	First Principles Simulations of the Electrochemical Lithiation and Delithiation of Faceted Crystalline Silicon. Journal of the American Chemical Society, 2012, 134, 14362-14374.	13.7	221
6	First-Principles Analysis of Defect Thermodynamics and Ion Transport in Inorganic SEI Compounds: LiF and NaF. ACS Applied Materials & Interfaces, 2015, 7, 18985-18996.	8.0	191
7	Enabling the high capacity of lithium-rich anti-fluorite lithium iron oxide by simultaneous anionic and cationic redox. Nature Energy, 2017, 2, 963-971.	39.5	140
8	On the Origin of Photoluminescence in Silicon Nanocrystals: Pressure-Dependent Structural and Optical Studies. Nano Letters, 2012, 12, 4200-4205.	9.1	133
9	Synthesis of borophane polymorphs through hydrogenation of borophene. Science, 2021, 371, 1143-1148.	12.6	129
10	First-Principles Analysis of Defect-Mediated Li Adsorption on Graphene. ACS Applied Materials & Interfaces, 2014, 6, 21141-21150.	8.0	120
11	Synthesis, Characterization, and Structural Modeling of Highâ€Capacity, Dual Functioning MnO₂ Electrode/Electrocatalysts for Liâ€O₂ Cells. Advanced Energy Materials, 2013, 3, 75-84.	19.5	111
12	Machine Learning Force Field Parameters from Ab Initio Data. Journal of Chemical Theory and Computation, 2017, 13, 4492-4503.	5.3	105
13	Towards First Principles-Based Prediction of Highly Accurate Electrochemical Pourbaix Diagrams. Journal of Physical Chemistry C, 2015, 119, 18177-18187.	3.1	97
14	Dopant Modulated Li Insertion in Si for Battery Anodes: Theory and Experiment. Journal of Physical Chemistry C, 2011, 115, 18916-18921.	3.1	84
15	Ab Initio-Based Bond Order Potential to Investigate Low Thermal Conductivity of Stanene Nanostructures. Journal of Physical Chemistry Letters, 2016, 7, 3752-3759.	4.6	80
16	Theory of Thermal Relaxation of Electrons in Semiconductors. Physical Review Letters, 2017, 119, 136602.	7.8	78
17	Machine Learning Classical Interatomic Potentials for Molecular Dynamics from First-Principles Training Data. Journal of Physical Chemistry C, 2019, 123, 6941-6957.	3.1	72
18	Visualizing Redox Dynamics of a Single Ag/AgCl Heterogeneous Nanocatalyst at Atomic Resolution. ACS Nano, 2016, 10, 3738-3746.	14.6	61

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19	Machine learning in scanning transmission electron microscopy. Nature Reviews Methods Primers, 2022, 2, .	21.2	59
20	Thermal Stability of Colloidal InP Nanocrystals: Small Inorganic Ligands Boost High-Temperature Photoluminescence. ACS Nano, 2014, 8, 977-985.	14.6	57
21	Imaging Catalytic Activation of CO₂ on Cu₂O (110): A First-Principles Study. Chemistry of Materials, 2018, 30, 1912-1923.	6.7	56
22	Surface Coverage and SEI Induced Electrochemical Surface Stress Changes during Li Deposition in a Model System for Li-Ion Battery Anodes. Journal of the Electrochemical Society, 2013, 160, A888-A896.	2.9	55
23	Origin and regulation of oxygen redox instability in high-voltage battery cathodes. Nature Energy, 2022, 7, 808-817.	39.5	55
24	Structure of Lithium Peroxide. Journal of Physical Chemistry Letters, 2011, 2, 2483-2486.	4.6	53
25	Machine learning on neutron and x-ray scattering and spectroscopies. Chemical Physics Reviews, 2021, 2, .	5.7	49
26	The First-Cycle Electrochemical Lithiation of Crystalline Ge: Dopant and Orientation Dependence and Comparison with Si. Journal of Physical Chemistry Letters, 2011, 2, 3092-3095.	4.6	48
27	Polar Fluctuations in Metal Halide Perovskites Uncovered by Acoustic Phonon Anomalies. ACS Energy Letters, 2017, 2, 2463-2469.	17.4	47
28	In situ high-energy synchrotron X-ray diffraction studies and first principles modeling of Î±-MnO₂ electrodes in Liâ€“O₂ and Li-ion coin cells. Journal of Materials Chemistry A, 2015, 3, 7389-7398.	10.3	43
29	Electronic structure of lithium battery interphase compounds: Comparison between inelastic x-ray scattering measurements and theory. Journal of Chemical Physics, 2011, 135, 224513.	3.0	39
30	Anharmonic stabilization and lattice heat transport in rocksalt Î²-GeTe. Applied Physics Letters, 2018, 113, .	3.3	39
31	Template-Free Vapor-Phase Growth of PatrÃ³nite by Atomic Layer Deposition. Chemistry of Materials, 2017, 29, 2864-2873.	6.7	37
32	Comprehensive Computational Study of Partial Lead Substitution in Methylammonium Lead Bromide. Chemistry of Materials, 2019, 31, 3599-3612.	6.7	37
33	Atomic and electronic structure of Lomer dislocations at CdTe bicrystal interface. Scientific Reports, 2016, 6, 27009.	3.3	35
34	Atomistic determination of the surface structure of Cu₂O(111): experiment and theory. Physical Chemistry Chemical Physics, 2018, 20, 27456-27463.	2.8	33
35	Effect of selenium and chlorine co-passivation in polycrystalline CdSeTe devices. Applied Physics Letters, 2019, 115, .	3.3	33
36	Slow Organicâ€toâ€Inorganic Subâ€Lattice Thermalization in Methylammonium Lead Halide Perovskites Observed by Ultrafast Photoluminescence. Advanced Energy Materials, 2016, 6, 1600422.	19.5	32

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37	Machine-learned impurity level prediction for semiconductors: the example of Cd-based chalcogenides. Npj Computational Materials, 2020, 6, .	8.7	32
38	Atomic scale study of polar Lomerâ€“Cottrell and Hirth lock dislocation cores in CdTe. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, 524-531.	0.1	31
39	Probing the Release and Uptake of Water in Î±-MnO₂Â·xH₂O. Chemistry of Materials, 2017, 29, 1507-1517.	6.7	31
40	Defect Evolution in Graphene upon Electrochemical Lithiation. ACS Applied Materials & Interfaces, 2014, 6, 17626-17636.	8.0	30
41	Computational prediction of lattice thermal conductivity: A comparison of molecular dynamics and Boltzmann transport approaches. Physical Review Materials, 2019, 3, .	2.4	29
42	Vision for Designing High-Energy, Hybrid Li Ion/Liâ€“O₂ Cells. Journal of Physical Chemistry Letters, 2013, 4, 3607-3611.	4.6	26
43	Describing the Diverse Geometries of Gold from Nanoclusters to Bulkâ€”A First-Principles-Based Hybrid Bond-Order Potential. Journal of Physical Chemistry C, 2016, 120, 13787-13800.	3.1	26
44	Lattice thermal transport in group II-alloyed PbTe. Applied Physics Letters, 2018, 112, .	3.3	26
45	Probing Electrochemically Induced Structural Evolution and Oxygen Redox Reactions in Layered Lithium Iridate. Chemistry of Materials, 2019, 31, 4341-4352.	6.7	26
46	Data-driven design of novel halide perovskite alloys. Energy and Environmental Science, 2022, 15, 1930-1949.	30.8	26
47	Understanding Polyol Decomposition on Bimetallic Ptâ€“Mo Catalystsâ€”A DFT Study of Glycerol. ACS Catalysis, 2015, 5, 4942-4950.	11.2	25
48	Slow thermal equilibration in methylammonium lead iodide revealed by transient mid-infrared spectroscopy. Nature Communications, 2018, 9, 2792.	12.8	25
49	Infrared-pump electronic-probe of methylammonium lead iodide reveals electronically decoupled organic and inorganic sublattices. Nature Communications, 2019, 10, 482.	12.8	25
50	Development of a Modified Embedded Atom Force Field for Zirconium Nitride Using Multi-Objective Evolutionary Optimization. Journal of Physical Chemistry C, 2016, 120, 17475-17483.	3.1	23
51	Evolutionary Optimization of a Charge Transfer Ionic Potential Model for Ta/Ta-Oxide Heterointerfaces. Chemistry of Materials, 2017, 29, 3603-3614.	6.7	22
52	Controlling Interfacial Properties of Lithiumâ€ion Battery Cathodes with Alkylphosphonate Selfâ€Assembled Monolayers. Advanced Materials Interfaces, 2018, 5, 1701292.	3.7	22
53	Universal machine learning framework for defect predictions in zinc blende semiconductors. Patterns, 2022, 3, 100450.	5.9	22
54	Unraveling the Planar-Globular Transition in Gold Nanoclusters through Evolutionary Search. Scientific Reports, 2016, 6, 34974.	3.3	21

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55	The Role of Water in the Reversible Optoelectronic Degradation of Hybrid Perovskites at Low Pressure. Journal of Physical Chemistry C, 2017, 121, 25659-25665.	3.1	19
56	Defect Energetics in Pseudo-Cubic Mixed Halide Lead Perovskites from First-Principles. Journal of Physical Chemistry C, 2020, 124, 16729-16738.	3.1	19
57	A scripting interface for GSAS-II. Journal of Applied Crystallography, 2018, 51, 1244-1250.	4.5	17
58	Identifying the Chemical Origin of Oxygen Redox Activity in Li-Rich Anti-Fluorite Lithium Iron Oxide by Experimental and Theoretical X-ray Absorption Spectroscopy. Journal of Physical Chemistry Letters, 2019, 10, 806-812.	4.6	17
59	Understanding the Role of Overpotentials in Lithium Ion Conversion Reactions: Visualizing the Interface. ACS Nano, 2019, 13, 7825-7832.	14.6	16
60	Two-Dimensional CsAg₅Te_{3â€“x}S_x Semiconductors: Multi-anion Chalcogenides with Dynamic Disorder and Ultralow Thermal Conductivity. Chemistry of Materials, 2018, 30, 7245-7254.	6.7	15
61	Direct Observation of Bandgap Oscillations Induced by Optical Phonons in Hybrid Lead Iodide Perovskites. Advanced Functional Materials, 2020, 30, 1907982.	14.9	15
62	Atomistic manipulation of reversible oxidation and reduction in Ag with an electron beam. Nanoscale, 2019, 11, 10756-10762.	5.6	14
63	Charge Transfer Dynamics of Phase-Segregated Halide Perovskites: CH₃NH₃PbCl₃ and CH₃NH₃PbI₃ or (C₄H₉NH₃)₂(CH₃NH₃)_{nâ^'1}Pbs Mixtures. ACS Applied Materials & Interfaces, 2019, 11, 9583-9593.	8.0	14
64	Quantitative Observation of Threshold Defect Behavior in Memristive Devices with Operando X-ray Microscopy. ACS Nano, 2018, 12, 4938-4945.	14.6	12
65	Mechanism of Na accumulation at extended defects in Si from first-principles. Journal of Applied Physics, 2018, 123, 161560.	2.5	12
66	Validating first-principles molecular dynamics calculations of oxide/water interfaces with x-ray reflectivity data. Physical Review Materials, 2020, 4, .	2.4	12
67	Ingrained: An Automated Framework for Fusing Atomicâ€Scale Image Simulations into Experiments. Small, 2022, 18, e2102960.	10.0	12
68	Machine learnt bond order potential to model metalâ€“organic (Coâ€“C) heterostructures. Nanoscale, 2017, 9, 18229-18239.	5.6	11
69	Operando Observations and Firstâ€Principles Calculations of Reduced Lithium Insertion in Auâ€Coated LiMn 2 O 4. Advanced Materials Interfaces, 2019, 6, 1801923.	3.7	11
70	UNCERTAINTY CLASSIFICATION AND VISUALIZATION OF MOLECULAR INTERFACES. , 2013, 3, 157-169.		10
71	Stabilization of a monolayer tellurene phase at CdTe interfaces. Nanoscale, 2019, 11, 14698-14706.	5.6	10
72	Accelerated screening of functional atomic impurities in halide perovskites using high-throughput computations and machine learning. Journal of Materials Science, 2022, 57, 10736-10754.	3.7	10

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73	Exploring the Origin of Anionic Redox Activity in Super Li-Rich Iron Oxide-Based High-Energy-Density Cathode Materials. Chemistry of Materials, 2022, 34, 4536-4547.	6.7	10
74	Ultrafast formation of a transient two-dimensional diamondlike structure in twisted bilayer graphene. Physical Review B, 2020, 102, .	3.2	8
75	Electronic transport in VO2â€"Experimentally calibrated Boltzmann transport modeling. Applied Physics Letters, 2015, 107, .	3.3	7
76	Polaron Structure and Transport in Fullerene Materials: Insights from First-Principles Calculations. Journal of Physical Chemistry C, 2014, 118, 21785-21797.	3.1	6
77	Enabling direct silicene integration in electronics: First principles study of silicene on NiSi2(111). Applied Physics Letters, 2016, 109, .	3.3	6
78	Study of Effects of Cl and Se in CdSeTe Solar Cells Using Scanning Transmission Electron Microscopy. Microscopy and Microanalysis, 2019, 25, 2150-2151.	0.4	5
79	Machine learning for impurity charge-state transition levels in semiconductors from elemental properties using multi-fidelity datasets. Journal of Chemical Physics, 2022, 156, 114110.	3.0	5
80	Spectroscopic Comparison of Thermal Transport at Organicâ€"Inorganic and Organic-Hybrid Interfaces Using CsPbBr₃ and FAPbBr₃ (FA = Formamidinium) Perovskite Nanocrystals. Nano Letters, 2019, 19, 8155-8160.	9.1	4
81	Fluoroethylene Carbonate Breakdown Mechanisms and Energetics on Two Lithium Silicide Surfaces. Journal of Physical Chemistry C, 2019, 123, 26743-26751.	3.1	4
82	A Two-Stage Framework for Compound Figure Separation. , 2021, , .		4
83	Atomistic simulations of grain boundaries in CdTe. , 2015, , .		3
84	An Autonomous Microscopy Workflow for Structure Determination from Atomic-Resolution Images. Microscopy and Microanalysis, 2018, 24, 510-511.	0.4	3
85	Atomic Scale Study of Lomer-Cottrell and Hirth Lock Dislocations in CdTe. Microscopy and Microanalysis, 2015, 21, 2087-2088.	0.4	2
86	Creation and analysis of atomic structures for CdTe bi-crystal interfaces by the grain boundary genie. , 2015, , .		2
87	Atomic-Resolution Study of Grain Boundaries in CdTe Using Scanning Transmission Electron Microscopy. Microscopy and Microanalysis, 2018, 24, 102-103.	0.4	2
88	Seebeck Tensor Analysis of (p Ã— n)-type Transverse Thermoelectric Materials. MRS Advances, 2019, 4, 491-497.	0.9	2
89	First principles modeling of polymer encapsulant degradation in Si photovoltaic modules. Physical Chemistry Chemical Physics, 2021, 23, 10357-10364.	2.8	2
90	4D >Crystal: Deep Learning Crystallographic Information From Electron Diffraction Images. Microscopy and Microanalysis, 2021, 27, 2774-2776.	0.4	2

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91	Computational design of passivants for CdTe grain boundaries. Solar Energy Materials and Solar Cells, 2021, 232, 111279.	6.2	2
92	Atomistic and First Principles: Computational Studies of LiO2 Batteries. , 2014, , 159-177.		2
93	Cu-Local Structures and Their Relation with Nanoscale Electrical Performance in CdTe. , 2020, , .		2
94	Leveraging First Principles Modeling and Machine Learning for Microscopy Data Inversion. Microscopy and Microanalysis, 2017, 23, 178-179.	0.4	1
95	Constructing Self-Labeled Materials Imaging Datasets from Open Access Scientific Journals with EXSCLAIM!. Microscopy and Microanalysis, 2020, 26, 3096-3097.	0.4	1
96	Unraveling Cu chemical signature in CdTe by Spectral Fluorescence Mapping. , 2021, , .		1
97	The Role of Water on the Interfacial Adhesion in Si Solar Modules. , 2021, , .		1
98	Open-Source Tools and Containers for the Production of Large-Scale S/TEM Datasets. Microscopy and Microanalysis, 2021, 27, 62-63.	0.4	1
99	A fundamental study of the effects of grain boundaries on performance of poly-crystalline thin film CdTe solar cells. , 2015, , .		0
100	Atomic â€" Scale study of model CdTe grain boundaries. , 2016, , .		0
101	First principles modeling of grain boundaries in CdTe. , 2016, , .		0
102	Atomistic Study of Model CdTe Grain Boundaries. Microscopy and Microanalysis, 2016, 22, 1398-1399.	0.4	0
103	Atomic â€" scale study of model CdTe grain boundaries. , 2017, , .		0
104	Study of Se and Cl segregation in poly-crystalline CdSeTe. , 2019, , .		0