Citation Report

List of articles citing

The Computational 2D Materials Database: high-throughput modeling and discovery of atomically thin crystals

#	Paper	IF	Citations
574	Stark shift of excitons and trions in two-dimensional materials. **2018**, 98,		14
573	Efficient Charge Separation in 2D Janus van der Waals Structures with Built-in Electric Fields and Intrinsic p🗆 Doping. **2018**, 122, 24520-24526		44
572	Uncovering a Stable Phase in Group V Transition-metal Dinitride (MN2, M = Ta, Nb, V) Nanosheets and Their Electronic Properties via First-principles Investigations. **2018**, 122, 26748-26755		15
571	Electronic excitations in transition metal dichalcogenide monolayers from an LDA+GdW approach. **2018**, 98,		25
570	Stacked Janus Device Concepts: Abrupt pn-Junctions and Cross-Plane Channels. **2018**, 18, 7275-7281		45
569	Recent advances and applications of machine learning in solid-state materials science. **2019**, 5,		631
568	The Computational Design of Two-Dimensional Materials. **2019**, 96, 2308-2314		6
567	Two-dimensional ferromagnetic materials and related van der Waals heterostructures: a first-principle study. **2019**, 40, 081509		3
566	Comment on 🗆he Computational 2D Materials Database: high-throughput modeling and discovery of atomically thin crystals🗆2D Materials, **2019**, 6, 048001	5.9	49
565	2D materials as an emerging platform for nanopore-based power generation. **2019**, 4, 588-605		120
564	Two-dimensional excitons in monolayer transition metal dichalcogenides from radial equation and variational calculations. **2019**, 31, 105702		7
563	Defect tolerant and dimension dependent ferromagnetism in MnSe. **2019**, 21, 16718-16725		13
562	Two-dimensional transition-metal halide CoBr with spin-polarized Dirac cone. **2019**, 21, 17740-17745		9
561	High throughput computational screening for 2D ferromagnetic materials: the critical role of anisotropy and local correlations. *2D Materials*, **2019**, 6, 045018	5.9	53
560	Classifying the Electronic and Optical Properties of Janus Monolayers. **2019**, 13, 13354-13364		43
559	Two-dimensional topological materials discovery by symmetry-indicator method. **2019**, 100,		17
558	Anisotropic Rashba effect and charge and spin currents in monolayer BiTeI by controlling symmetry. **2019**, 100,		9

539 First-principles investigation on hydrogen evolution reaction in KNbO3 (100)/g-C3N4 heterojunction. **2019**, 582, 117103 — 5

538 Hexagonal CuCl Monolayer for Water Splitting: A DFT Study. **2019**, 2, 4238-4246 — 10

537 Stable Two-Dimensional Materials for Oxygen Reduction and Oxygen Evolution Reactions. **2019**, 4, 1410-1411 — 33

536 Dimension engineering of single-layer PtN 2 with the Cairo tessellation. **2019**, 125, 204302 — 1

535 The Compendium: A Practical Guide to Theoretical Photoemission Spectroscopy. **2019**, 7, 377 — 139

534 Production of large-area 2D materials for high-performance photodetectors by pulsed-laser deposition. **2019**, 106, 100573 — 94

533 Catalysis-Hub.org, an open electronic structure database for surface reactions. **2019**, 6, 75 — 88

532 Enhancing and Controlling Plasmons in Janus MoSSeΓraphene Based van der Waals Heterostructures. **2019**, 123, 16373-16379 — 16

531 2DMatPedia, an open computational database of two-dimensional materials from top-down and bottom-up approaches. **2019**, 6, 86 — 92

530 Computational prediction and characterization of two-dimensional pentagonal arsenopyrite FeAsS. **2019**, 166, 105-110 — 5

529 The origin of intrinsic charge transport for Dirac carbon sheet materials: roles of acetylenic linkage and electron-phonon couplings. **2019**, 11, 10828-10837 — 6

528 Machine Learning for Computational Heterogeneous Catalysis. **2019**, 11, 3581-3601 — 127

527 Spontaneous breaking of time-reversal symmetry at the edges of 1T? monolayer transition metal dichalcogenides. **2019**, 99, — 3

526 Energy, Phonon, and Dynamic Stability Criteria of Two-Dimensional Materials. **2019**, 11, 24876-24884 — 33

525 A New Family of Two-Dimensional Crystals: Open-Framework T X (T = C, Si, Ge, Sn; X = O, S, Se, Te) Compounds with Tetrahedral Bonding. **2019**, 19, 2694-2699 — 7

524 Prediction of Synthesis of 2D Metal Carbides and Nitrides (MXenes) and Their Precursors with Positive and Unlabeled Machine Learning. **2019**, 13, 3031-3041 — 95

523 Finite-momentum exciton landscape in mono- and bilayer transition metal dichalcogenides. *2D Materials*, **2019**, 6, 035003 — 5.9 — 51

522 Out-of-plane excitons in two-dimensional crystals. **2019**, 99, — 17

521   From DFT to machine learning: recent approaches to materials science a review. **2019**, 2, 032001   206

520   Beyond the RPA and GW methods with adiabatic xc-kernels for accurate ground state and quasiparticle energies. **2019**, 5,   19

519   Edge, size, and shape effects on WS, WSe, and WTe nanoflake stability: design principles from an ab initio investigation. **2019**, 21, 23076-23084   11

518   Topological flat band, Dirac fermions and quantum spin Hall phase in 2D Archimedean lattices. **2019**, 21, 22344-22350   22

517   First-Principles Exploration of Two-Dimensional Transition Metal Dichalcogenides Based on Fe, Co, Ni, and Cu Groups and Their van der Waals Heterostructures. **2019**, 2, 8491-8501   12

516   Electrically-Transduced Chemical Sensors Based on Two-Dimensional Nanomaterials. **2019**, 119, 478-598   294

515   Calculating critical temperatures for ferromagnetic order in two-dimensional materials. *2D Materials*, **2019**, 6, 015028   5.9   64

514   From pentagonal geometries to two-dimensional materials. **2019**, 159, 448-453   15

513   Towards photoferroic materials by design: recent progress and perspectives. **2020**, 2, 011001   7

512   2D Electrocatalysts for Converting Earth-Abundant Simple Molecules into Value-Added Commodity Chemicals: Recent Progress and Perspectives. **2020**, 32, e1904870   49

511   Materials selection rules for optimum power factor in two-dimensional thermoelectrics. **2020**, 3, 015005   3

510   Large-Spin-Gap Nodal-Line Half-Metal and High-Temperature Ferromagnetic Semiconductor in Cr2X3 (X=O,S,Se) Monolayers. **2020**, 6, 1900490   15

509   Exploring Two-Dimensional Materials Thermodynamic Stability via Machine Learning. **2020**, 12, 20149-20157   43

508   Visible-blind UV-Detector properties of monolayer calcium chloride: DFT calculations of its structural, mechanical, electronic and optical properties. **2020**, 306, 113771   2

507   Simulations and Materials Chemistry in the Age of Big Data. **2020**, 60, 452-459   18

506   First-principles calculations of charge carrier mobility and conductivity in bulk semiconductors and two-dimensional materials. **2020**, 83, 036501   71

505   High throughput study on magnetic ground states with Hubbard U corrections in transition metal dihalide monolayers. **2020**, 2, 495-501   9

504   Optoelectronic and photonic devices based on transition metal dichalcogenides. **2020**, 7, 014002   31

| 503 | Excited-State Properties of Janus Transition-Metal Dichalcogenides. **2020**, 124, 1667-1673 | 8 |

| 502 | Electronic Polarizability as the Fundamental Variable in the Dielectric Properties of Two-Dimensional Materials. **2020**, 20, 841-851 | 31 |

| 501 | Intercalation-Driven Reversible Switching of 2D Magnetism. **2020**, 124, 1146-1157 | 6 |

| 500 | High-Throughput Computational Characterization of 2D Compositionally Complex Transition-Metal Chalcogenide Alloys. **2020**, 3, 2000195 | 2 |

| 499 | Beyond Graphene: Low-Symmetry and Anisotropic 2D Materials. **2020**, 128, 140401 | 5 |

| 498 | Quantum anomalous Hall effect in two-dimensional magnetic insulator heterojunctions. **2020**, 6, | 11 |

| 497 | High-throughput computational screening for two-dimensional magnetic materials based on experimental databases of three-dimensional compounds. **2020**, 6, | 15 |

| 496 | Model Hamiltonian for the Quantum Anomalous Hall State in Iron-Halogenide. **2020**, 37, 097301 | 4 |

| 495 | A Theoretical Analysis on the Oxidation and Water Dissociation Resistance on Group-IV Phosphide Monolayers. **2020**, 21, 2539-2549 | 10 |

| 494 | Determining dimensionalities and multiplicities of crystal nets. **2020**, 6, | 2 |

| 493 | Tunable valley polarization, magnetic anisotropy and Dzyaloshinskii-Moriya interaction in two-dimensional intrinsic ferromagnetic Janus 2H-VSeX (X = S, Te) monolayers. **2020**, 22, 23597-23608 | 14 |

| 492 | Two-dimensional gallium and indium oxides from global structure searching: Ferromagnetism and half metallicity via hole doping. **2020**, 128, 034304 | 4 |

| 491 | Femtosecond exciton dynamics in WSe optical waveguides. **2020**, 11, 3567 | 13 |

| 490 | Boron nitride switches for 5G and beyond. **2020**, 3, 444-445 | 2 |

| 489 | Machine learning-driven new material discovery. **2020**, 2, 3115-3130 | 30 |

| 488 | Computational Screening of Atomically Thin Two-Dimensional Nanomaterial-Coated Cs3Sb Heterostructures for High-Performance Photocathodes. **2020**, 124, 26396-26403 | 2 |

| 487 | Crystal Structure Prediction of Binary Alloys via Deep Potential. **2020**, 8, 589795 | 4 |

| 486 | Engineering Dielectric Screening for Potential-well Arrays of Excitons in 2D Materials. **2020**, 12, 55134-55140 | 4 |

485   Tuplewise Material Representation Based Machine Learning for Accurate Band Gap Prediction. **2020**, 124, 10616-10623   11

484   Spin orientation and strain tuning valley polarization with magneto-optic Kerr effects in ferrovalley VS2 monolayer. **2020**, 117, 042406   5

483   Optical Gaps and Excitonic Properties of 2D Materials by Hybrid Time-Dependent Density Functional Theory: Evidences for Monolayers and Prospects for van der Waals Heterostructures. **2020**, 16, 5876-5883   10

482   The Pair Approximation method for the ferromagnetic Heisenberg model with spin S=1 and arbitrary range of interactions. Application for the magnetic semiconductor CrIAs. **2020**, 513, 167157   1

481   Electronic-structure methods for twisted moirélayers. **2020**, 5, 748-763   51

480   Two-dimensional forms of robust CO_2 reduction photocatalysts. **2020**, 4,   9

479   Electronic Structure Based Intuitive Design Principle of Single-Atom Catalysts for Efficient Electrolytic Nitrogen Reduction. **2020**, 12, 5456-5464   10

478   Fabrication of 2D Crystals by Intercalation of a Bulk ZnWO4 Single Crystals. **2020**,

477   An artificial intelligence-aided virtual screening recipe for two-dimensional materials discovery. **2020**, 6,   14

476   Half-MetalSpin-Gapless-Semiconductor Junctions as a Route to the Ideal Diode. **2020**, 14,   9

475   Database of Two-Dimensional Hybrid Perovskite Materials: Open-Access Collection of Crystal Structures, Band Gaps, and Atomic Partial Charges Predicted by Machine Learning. **2020**, 32, 7383-7388   44

474   Blue Phosphorene Bilayer Is a Two-Dimensional Metal and an Unambiguous Classification Scheme for Buckled Hexagonal Bilayers. **2020**, 125, 196401   7

473   High-throughput computational screening of 2D materials for thermoelectrics. **2020**, 8, 19674-19683   10

472   Electrical Control of Spin-Injection Using Mixed Dimensional van der Waals Heterostructures. **2020**, 19, 736-743

471   Anisotropic Thermoelectric Power Factor of Two-Dimensional Materials with Periodic Potential Barriers: The Wigner-Rode Formalism. **2020**, 14,   1

470   Machine Learning-Enabled Design of Point Defects in 2D Materials for Quantum and Neuromorphic Information Processing. **2020**, 14, 13406-13417   28

469   Coulomb-engineered heterojunctions and dynamical screening in transition metal dichalcogenide monolayers. **2020**, 102,   3

468   Anisotropic properties of monolayer 2D materials: An overview from the C2DB database. **2020**, 128, 105101   6

467	A predictive model for high-frequency operation of two-dimensional transistors from first-principles. **2020**, 128, 234502		3
466	Anomalous exciton Rydberg series in two-dimensional semiconductors on high-dielectric substrates. **2020**, 102,		4
465	Interplay between spin proximity effect and charge-dependent exciton dynamics in MoSe/CrBr van der Waals heterostructures. **2020**, 11, 6021		22
464	First-principles prediction of a room-temperature ferromagnetic and ferroelastic 2D multiferroic MnNX (X = F, Cl, Br, and I). **2020**, 12, 24237-24243		7
463	Erratum: Accurate electronic band gaps of two-dimensional materials from the local modified Becke-Johnson potential [Phys. Rev. B 101, 245163 (2020)]. **2020**, 102,		4
462	Electronic structure calculations of twisted multi-layer graphene superlattices. *2D Materials*, **2020**, 7, 035028	5.9	15
461	Magneto-optical response of chromium trihalide monolayers: chemical trends. **2020**, 8, 8856-8863		14
460	Efficient Ab Initio Modeling of Dielectric Screening in 2D van der Waals Materials: Including Phonons, Substrates, and Doping. **2020**, 124, 11609-11616		12
459	Engineering covalently bonded 2D layered materials by self-intercalation. **2020**, 581, 171-177		68
458	Amorphization of Indirect Band Gap Semiconductors To Tune Their Optoelectronic Properties. **2020**, 124, 14432-14438		2
457	Ab Initio Studies of Exciton g Factors: Monolayer Transition Metal Dichalcogenides in Magnetic Fields. **2020**, 124, 226402		18
456	Hexagonal layered group IV-VI semiconductors and derivatives: fresh blood of the 2D family. **2020**, 12, 13450-13459		8
455	Structural Transition in Oxidized Ca2N Electrenes: CaO/CaN 2D Heterostructures. **2020**, 124, 14706-14712		0
454	Changes of Structure and Bonding with Thickness in Chalcogenide Thin Films. **2020**, 32, e2001033		7
453	Coupling a Crystal Graph Multilayer Descriptor to Active Learning for Rapid Discovery of 2D Ferromagnetic Semiconductors/Half-Metals/Metals. **2020**, 32, e2002658		36
452	A library of ab initio Raman spectra for automated identification of 2D materials. **2020**, 11, 3011		17
451	Towards elucidating structure of ligand-protected nanoclusters. **2020**, 49, 9191-9202		8
450	First-principles investigation of ScX (X = Cl, Br, or I) monolayers for flexible spintronic and electronic applications. **2020**, 22, 14781-14786		2

449   LAN: A Materials Notation for Two-Dimensional Layered Assemblies. **2020**, 60, 3457-3462   2

448   Room Temperature Terahertz Electroabsorption Modulation by Excitons in Monolayer Transition Metal Dichalcogenides. **2020**, 20, 5214-5220   2

447   Semiconducting few-layer PdSe and PdSe: native point defects and contacts with native metallic PdSe. **2020**, 22, 7365-7373   4

446   Electrically controlled dielectric band gap engineering in a two-dimensional semiconductor. **2020**, 101,   7

445   Ferroelectricity and multiferroicity in two-dimensional ScPSe and ScCrPSe monolayers. **2020**, 22, 7489-7496   9

444   Monolayer diboron dinitride: Direct band-gap semiconductor with high absorption in the visible range. **2020**, 101,   6

443   Engineering Metal-sp Dirac Bands on the Oxidized SiC Surface. **2020**, 20, 3956-3962   4

442   Light-matter interaction in van der Waals hetero-structures. **2020**, 32, 333002   6

441   Activation of topological insulator phase in kagome-type bilayers by interlayer coupling: The cases of Ni(CO)4 and Pd(CO)4. **2020**, 116, 103103   2

440   High oscillator strength interlayer excitons in two-dimensional heterostructures for mid-infrared photodetection. **2020**, 15, 675-682   56

439   Accurate electronic band gaps of two-dimensional materials from the local modified Becke-Johnson potential. **2020**, 101,   8

438   AlN and GaN Nanostructures: Analytical Estimations of the Characteristics of the Electronic Spectrum. **2020**, 62, 1085-1089   1

437   Generalized Scaling Law for Exciton Binding Energy in Two-Dimensional Materials. **2020**, 13,   7

436   Efficient Method for Modeling Polarons Using Electronic Structure Methods. **2020**, 16, 5264-5278   16

435   Optical spectra of 2D monolayers from time-dependent density functional theory. **2020**, 224, 467-482   3

434   Thermochemical stability, and electronic and dielectric properties of Janus bismuth oxyhalide BiOX (X = Cl, Br, I) monolayers. **2020**, 2, 1090-1104   8

433   Electronic and optical properties of zinc based hybrid organic-inorganic compounds. **2020**, 7, 035701   5

432   Phonon-Assisted Photoluminescence from Indirect Excitons in Monolayers of Transition-Metal Dichalcogenides. **2020**, 20, 2849-2856   51

431	Computational functionality-driven design of semiconductors for optoelectronic applications. **2020**, 2, 879-904		19
430	Local Modified Becke-Johnson Exchange-Correlation Potential for Interfaces, Surfaces, and Two-Dimensional Materials. **2020**, 16, 2654-2660		15
429	Catalytic Activity and Stability of Two-Dimensional Materials for the Hydrogen Evolution Reaction. **2020**, 5, 885-891		22
428	Autonomous Discovery of Materials for Intercalation Electrodes. **2020**, 3, 488-498		15
427	Structural and electronic properties of two-dimensional hydrogenated Xenes. **2020**, 32, 205501		5
426	Growing field of materials informatics: databases and artificial intelligence. **2020**, 10, 1-10		5
425	Production and processing of graphene and related materials. *2D Materials*, **2020**, 7, 022001	5.9	179
424	Two-dimensional MXenes: From morphological to optical, electric, and magnetic properties and applications. **2020**, 848, 1-58		321
423	Strong Light‑Matter Interactions Enabled by Polaritons in Atomically Thin Materials. **2020**, 8, 1901473		30
422	Atomistic T-matrix theory of disordered two-dimensional materials: Bound states, spectral properties, quasiparticle scattering, and transport. **2020**, 101,		7
421	Proximity Effect in Crystalline Framework Materials: Stacking-Induced Functionality in MOFs and COFs. **2020**, 30, 1908004		36
420	Status and Future Prospects of CMOS Scaling and Moore's Law - A Personal Perspective. **2020**,		3
419	Engineering Atomically Sharp Potential Steps and Band Alignment at Solid Interfaces using 2D Janus Layers. **2020**, 124, 9572-9580		5
418	Structural stability of single-layer PdSe with pentagonal puckered morphology and its nanotubes. **2020**, 22, 8289-8295		9
417	Emergence of d-orbital magnetic Dirac fermions in a MoS2 monolayer with squared pentagon structure. **2020**, 101,		3
416	Conductance of quantum spin Hall edge states from first principles: The critical role of magnetic impurities and inter-edge scattering. **2020**, 101,		8
415	Effects of Components Modulation on the Type of Band Alignments for PbI2/WS2 van der Waals Heterostructure. **2020**, 14, 2000016		19
414	Atomically scale design of van der Waals heterostructures as photocatalysts. **2020**, 511-525		0

413	Strategies for designing two-dimensional nonlinear optical layers from KBBF and BBO crystals. **2020**, 5, 985-995		4
412	High-throughput discovery of high Curie point two-dimensional ferromagnetic materials. **2020**, 6,		35
411	Catalyst Acquisition by Data Science (CADS): a web-based catalyst informatics platform for discovering catalysts. **2020**, 5, 903-911		15
410	Excellent electronic transport in heterostructures of graphene and monoisotopic boron-nitride grown at atmospheric pressure. *2D Materials*, **2020**, 7, 031009	5.9	11
409	Germanene/2D-SiC van der Waals heterobilayer: Structural features and tunable electronic properties. **2021**, 26, 101718		10
408	Structure prediction of two-dimensional materials based on neural network-driven evolutionary technique. **2021**, 186, 110046		
407	Intrinsic mechanical properties of monolayer nickel ditelluride: An atomistic study. **2021**, 26, e00522		1
406	Liquid Exfoliated SnP3 Nanosheets for Very High Areal Capacity Lithium-Ion Batteries. **2021**, 11, 2002364		17
405	Two-dimensional MX Dirac materials and quantum spin Hall insulators with tunable electronic and topological properties. **2021**, 14, 584-589		5
404	Large family of two-dimensional ferroelectric metals discovered via machine learning. **2021**, 66, 233-242		15
403	Review: Simulation Models for Materials and Biomolecules. **2021**, 27-82		1
402	A structure map for AB2 type 2D materials using high-throughput DFT calculations. **2021**, 2, 4392-4413		4
401	Two-dimensional C3N/blue phosphorene vdW heterostructure for Li, Na and K-ion batteries. **2021**, 45, 12647-12654		2
400	Ultralow lattice thermal conductivity and dramatically enhanced thermoelectric properties of monolayer InSe induced by an external electric field. **2021**, 23, 13633-13646		2
399	Me-graphane: tailoring the structural and electronic properties of Me-graphene hydrogenation. **2021**, 23, 9483-9491		5
398	Metastable piezoelectric group-IV monochalcogenide monolayers with a buckled honeycomb structure. **2021**, 103,		4
397	Two-dimensional Weyl points and nodal lines in pentagonal materials and their optical response. **2021**, 13, 6117-6128		1
396	Ab initio perspective of ultra-scaled CMOS from 2D-material fundamentals to dynamically doped transistors. **2021**, 5,		6

395	Synergistic vacancy defects and mechanical strain for the modulation of the mechanical, electronic and optical properties of monolayer tungsten disulfide. **2021**, 23, 6298-6308	1
394	Computational Screening of Photocathodes Based on Layered MXene coated Cs3Sb Heterostructures. **2021**, 0-0	
393	Flexoelectricity in atomic monolayers from first principles. **2021**, 13, 1600-1607	17
392	Towards fully automated GW band structure calculations: What we can learn from 60.000 self-energy evaluations. **2021**, 7,	3
391	Induced half-metallic characteristics and enhanced magnetic anisotropy in the two-dimensional Janus VIBr monolayer by graphyne adsorption. **2021**, 23, 17338-17347	2
390	First-principles discovery of stable two-dimensional materials with giant piezoelectric response. **2020**,	0
389	Computational design of a polymorph for 2D III-V orthorhombic monolayers by first principles calculations: excellent anisotropic, electronic and optical properties. **2021**, 23, 3771-3778	5
388	Predicting the Electronic and Structural Properties of Two-Dimensional Materials Using Machine Learning. **2021**, 67, 1287-1300	1
387	Full quantum search for high T two-dimensional van der Waals ferromagnetic semiconductors. **2021**, 13, 8137-8145	3
386	Design of a noble-metal-free direct Z-scheme photocatalyst for overall water splitting based on a SnC/SnSSe van der Waals heterostructure. **2021**, 23, 21641-21651	2
385	MoS2 and Janus (MoSSe) based 2D van der Waals heterostructures: emerging direct Z-scheme photocatalysts. **2021**, 3, 2837-2845	5
384	Schottky barrier lowering due to interface states in 2D heterophase devices. **2021**, 3, 567-574	4
383	Constructing two-dimensional materials at atomic scale from a theoretical perspective. **2021**, 0-0	2
382	Exfoliation of boron carbide into ultrathin nanosheets. **2021**, 13, 1652-1662	8
381	The performance limits of hexagonal boron nitride as an insulator for scaled CMOS devices based on two-dimensional materials. **2021**, 4, 98-108	53
380	Anisotropic correlation between the piezoelectricity and anion-polarizability difference in 2D phosphorene-type ternary GaXY (X = Se, Te; Y = F, Cl, Br, I) monolayers. **2021**, 56, 8024-8036	4
379	Half-auxetic effect and ferroelasticity in a two-dimensional monolayer TiSe. **2021**,	1
378	High-throughput bandstructure simulations of van der Waals hetero-bilayers formed by 1T and 2H monolayers. **2021**, 5,	4

359	Scalable Synthesis of Atomically Thin Gallium Telluride Nanosheets for Supercapacitor Applications. **2021**, 4, 4829-4838	15
358	Discovery of higher-order topological insulators using the spin Hall conductivity as a topology signature. **2021**, 7,	2
357	Valley polarization, magnetic anisotropy and Dzyaloshinskii-Moriya interaction of two-dimensional graphene/Janus 2H-VSeX (X = S, Te) heterostructures. **2021**, 174, 540-555	16
356	A difference method with semi-analytical approach for achieving accuracy in optical gaps of 2D materials using exciton model in fractional space. **2021**, 60, 060905	1
355	Magnetic anisotropy and exchange interactions of two-dimensional FePS3, NiPS3 and MnPS3 from first principles calculations. **2021**, 54, 314001	6
354	An ab-initio study of 2 dimensional metal (Cu, Ag) - 1T[ReS2 van der Waals heterostructure. **2021**,	
353	Electronic-structure methods for materials design. **2021**, 20, 736-749	24
352	Theoretical study of structural and electronic properties of 2H-phase transition metal dichalcogenides. **2021**, 103,	2
351	Efficient Band Structure Calculation of Two-Dimensional Materials from Semilocal Density Functionals. **2021**, 125, 11206-11215	2
350	Predicting anomalous quantum confinement effect in van der Waals materials. **2021**, 5,	3
349	Combining density functional theory with macroscopic QED for quantum light-matter interactions in 2D materials. **2021**, 12, 2778	2
348	Second-Order Nonlinear Optical Properties of Monolayer Transition-Metal Dichalcogenides by Computational Analysis. **2021**, 125, 11075-11084	5
347	Optical emission from light-like and particle-like excitons in monolayer transition metal dichalcogenides. **2021**, 103,	3
346	Spectrum of Exfoliable 1D van der Waals Molecular Wires and Their Electronic Properties. **2021**, 15, 9851-9859	1
345	Mirror Chern numbers in the hybrid Wannier representation. **2021**, 103,	0
344	Computational Discovery of New 2D Materials Using Deep Learning Generative Models. **2021**, 13, 53303-53313	5
343	Two-dimensional black phosphorus: Properties, fabrication and application for flexible supercapacitors. **2021**, 412, 128744	10
342	Database Construction for Two-Dimensional Material-Substrate Interfaces. **2021**, 38, 066801	2

341	Machine learning approaches for feature engineering of the crystal structure: Application to the prediction of the formation energy of cubic compounds. **2021**, 5,	1
340	Two-Dimensional Chromium Bismuthate: A Room-Temperature Ising Ferromagnet with Tunable Magneto-Optical Response. **2021**, 15,	3
339	Opening band gaps of low-dimensional materials at the meta-GGA level of density functional approximations. **2021**, 5,	8
338	Magnus Hall Effect in Two-Dimensional Materials. **2021**, 38, 057301	1
337	Methods to accelerate high-throughput screening of atomic qubit candidates in van der Waals materials. **2021**, 129, 225105	1
336	Phonoritons as Hybridized Exciton-Photon-Phonon Excitations in a Monolayer h-BN Optical Cavity. **2021**, 126, 227401	4
335	Accessing the spectral function of in operando devices by angle-resolved photoemission spectroscopy. **2021**, 3, 021101	3
334	Accelerated discovery of a large family of quaternary chalcogenides with very low lattice thermal conductivity. **2021**, 7,	7
333	Benchmarking graph neural networks for materials chemistry. **2021**, 7,	20
332	Intraband Lifshitz transition and Stoner ferromagnetism in Janus PA2As (A=Si,Ge,Sn, and Pb) monolayers. **2021**, 104,	1

331	Two-dimensional binary metal-oxide quasicrystal approximants. *2D Materials*, **2021**, 8, 045002	5.9	1

330	Structure and Energetics of Dye-Sensitized NiO Interfaces in Water from Ab Initio MD and Large-Scale GW Calculations. **2021**, 17, 5225-5238	4
329	Reconstructing the exit wave in high-resolution transmission electron microscopy using machine learning. **2021**, 27, 254-256	0
328	Synthesis and Properties of Monolayer MnSe with Unusual Atomic Structure and Antiferromagnetic Ordering. **2021**,	2
327	Universal Scalings in Two-Dimensional Anisotropic Dipolar Excitonic Systems. **2021**, 127, 047402	3
326	Metastability relationship between two- and three-dimensional crystal structures: a case study of the Cu-based compounds. **2021**, 11, 14588	2
325	The data-intensive scientific revolution occurring where two-dimensional materials meet machine learning. **2021**, 2, 100482	6

324	Recent progress of the computational 2D materials database (C2DB). *2D Materials*, **2021**, 8, 044002	5.9	33

| 323 | Prediction of the two-dimensional Janus ferrovalley material LaBrI. **2021**, 104, | 5 |

| 322 | Concurrence of negative in-plane piezoelectricity and photocatalytic properties in 2D ScAgP2S6 monolayers. **2021**, 33, 375301 | 1 |

| 321 | Bounds on the in-plane Poisson's ratios and the in-plane linear and area compressibilities for sheet crystals. **2021**, 152, 104409 | 3 |

| 320 | High-throughput computational design for 2D van der Waals functional heterostructures: Fragility of Anderson's rule and beyond. **2021**, 119, 043102 | 10 |

| 319 | Bandgap prediction of two-dimensional materials using machine learning. **2021**, 16, e0255637 | 1 |

| 318 | Computational Exploration of Stable 4d/5d Transition-Metal MSi2N4 (M = Y‐d and Hf‐Ig) Nanosheets and Their Versatile Electronic and Magnetic Properties. **2021**, 125, 19580-19591 | 3 |

| 317 | Transport properties in partially overlapping van der Waals junctions through a multiscale investigation. **2021**, 104, | 3 |

| 316 | Integration of data-intensive, machine learning and robotic experimental approaches for accelerated discovery of catalysts in renewable energy-related reactions. **2021**, 1, 100049 | 2 |

| 315 | Single-Layer Zirconium Dihalides ZrX (X = Cl, Br, and I) with Abnormal Ferroelastic Behavior and Strong Anisotropic Light Absorption Ability. **2021**, 12, 7726-7732 | 3 |

| 314 | Shear and Breathing Modes of Layered Materials. **2021**, | 4 |

| 313 | Identification of two-dimensional layered dielectrics from first principles. **2021**, 12, 5051 | 13 |

| 312 | Flexible Piezoelectricity of Two-Dimensional Materials Governed by Effective Berry Curvature. **2021**, 12, 8220-8228 | 0 |

| 311 | Ten Years of Progress in the Synthesis and Development of MXenes. **2021**, 33, e2103393 | 91 |

| 310 | A density-functional-theory-based and machine-learning-accelerated hybrid method for intricate system catalysis. **2021**, 1, 100046 | 4 |

| 309 | Tunable effective masses of magneto-excitons in two-dimensional materials. **2021**, 334-335, 114371 | 0 |

| 308 | Torsional strain engineering of transition metal dichalcogenide nanotubes: anstudy. **2021**, 32, | 2 |

| 307 | Computational synthesis of substrates by crystal cleavage. **2021**, 7, | 1 |

| 306 | Spread-balanced Wannier functions: Robust and automatable orbital localization. **2021**, 104, | |

305	Machine learning for materials discovery: Two-dimensional topological insulators. **2021**, 8, 031409	7
304	Physical insights on transistors based on lateral heterostructures of monolayer and multilayer PtSe via Ab initio modelling of interfaces. **2021**, 11, 18482	1
303	High-throughput design of magnetic materials. **2021**, 3, 033001	4
302	Computational design of moirḗ assemblies aided by artificial intelligence. **2021**, 8, 031401	1
301	Feature Blending: An Approach toward Generalized Machine Learning Models for Property Prediction.	1
300	Bandgap of two-dimensional materials: Thorough assessment of modern exchange-correlation functionals. **2021**, 155, 104103	4
299	Low thermal conductivity: fundamentals and theoretical aspects in thermoelectric applications. **2021**, 21, 100744	13
298	Data-Driven Discovery of 2D Materials for Solar Water Splitting. **2021**, 8,	1
297	Investigation into thermoelectric properties of M (M=Hf, Zr) X2(X=S, Se, Te) nanotubes using first-principles calculation. **2021**, 336, 114289	1
296	First-principles calculations to investigate electronic structure and transport properties of CrC monolayers: A new horizon for spintronic application. **2021**, 272, 115379	1
295	Novel electronic structures and magnetic properties in twisted two-dimensional graphene/Janus 2H VSeTe heterostructures. **2021**, 134, 114854	3
294	Electronic properties of SrFCl and SrFBr monolayers using density functional theory and GW approximation. **2021**, 336, 114430	0
293	VASPKIT: A user-friendly interface facilitating high-throughput computing and analysis using VASP code. **2021**, 267, 108033	434
292	Atomic Simulation Recipes A Python framework and library for automated workflows. **2021**, 199, 110731	8
291	Accurate first-principles evaluation of structural, electronic, optical and photocatalytic properties of BaHfO3 and SrHfO3 perovskites. **2022**, 892, 162071	0
290	Prediction of allotropes of tellurium with molecular, one- and two-dimensional covalent nets for photofunctional applications.. **2021**, 11, 29965-29975	1
289	Group-IV(A) Janus dichalcogenide monolayers and their interfaces straddle gigantic shear and in-plane piezoelectricity. **2021**, 13, 5460-5478	29
288	Physics of electron emission and injection in two-dimensional materials: Theory and simulation. **2021**, 3, 502-535	19

287	Phase diagram exploration of Tc-Al-B: from bulk TcAlB to two-dimensional TcB. **2021**, 23, 22086-22095		
286	Towards the object-oriented design of active hydrogen evolution catalysts on single-atom alloys. **2021**, 12, 10634-10642		4
285	Band structure of MoSTe Janus nanotubes. **2021**, 5,		11
284	Group 11 Transition-Metal Halide Monolayers: High Promises for Photocatalysis and Quantum Cutting. **2021**, 12, 525-531		7
283	Data-driven studies of magnetic two-dimensional materials. **2020**, 10, 15795		10
282	Magnetic i-MXenes: a new class of multifunctional two-dimensional materials. **2020**, 12, 5995-6001		20
281	First principles Heisenberg models of 2D magnetic materials: the importance of quantum corrections to the exchange coupling. **2020**, 32, 335802		6
280	LCAO-TDDFT-k-▯ spectroscopy in the optical limit. **2020**, 32, 415901		2
279	Microscopic Coulomb interaction in transition-metal dichalcogenides. **2020**,		2
278	Widely tunable direct bandgap of two-dimensional GeSe. **2020**, 33, 115301		1
277	Bending moduli for forty-four select atomic monolayers from first principles. **2020**, 31, 43LT01		12
276	Electronic and optical properties of transition metal dichalcogenides under symmetric and asymmetric field-effect doping. **2020**, 22, 083072		2
275	Machine learning in materials design: Algorithm and application. **2020**, 29, 116103		11
274	An outlook into the flat land of 2D materials beyond graphene: synthesis, properties and device applications. *2D Materials*, **2021**, 8, 013001	5.9	12
273	Bending rigidities and universality of flexural modes in 2D crystals. **2020**, 3, 02LT03		0
272	Machine learning enabled discovery of application dependent design principles for two-dimensional materials. **2020**, 1, 035015		2
271	PtP2: An example of exploring the hidden Cairo tessellation in the pyrite structure for discovering novel two-dimensional materials. **2018**, 2,		10
270	Discovering two-dimensional topological insulators from high-throughput computations. **2019**, 3,		38

269   Definition of a scoring parameter to identify low-dimensional materials components. **2019**, 3,   12

268   Electronic and optical excitations of two-dimensional ZrS2 and HfS2 and their heterostructure. **2019**, 3,   11

267   Vibrational and dielectric properties of monolayer transition metal dichalcogenides. **2019**, 3,   7

266   Transferable screened range-separated hybrids for layered materials: The cases of MoS2 and h-BN. **2019**, 3,   10

265   Computational screening of two-dimensional coatings for semiconducting photocathodes. **2020**, 4,   5

264   Ferromagnetism and half-metallicity in two-dimensional MO (M=Ga,In) monolayers induced by hole doping. **2020**, 4,   5

263   Tuning hydrogen adsorption and electronic properties from graphene to fluorographone. **2020**, 4,   4

262   MoTe2 as a natural hyperbolic material across the visible and the ultraviolet region. **2020**, 4,   6

261   Spin-orbit-proximitized ferromagnetic metal by monolayer transition metal dichalcogenide: Atlas of spectral functions, spin textures, and spin-orbit torques in Co/MoSe2, Co/WSe2, and Co/TaSe2 heterostructures. **2020**, 4,   5

260   2D materials integrated with metallic nanostructures: fundamentals and optoelectronic applications. **2020**, 9, 1877-1900   16

259   MyQueue: Task and workflow scheduling system. **2020**, 5, 1844   20

258   Interlayer Exciton in Transition Metal Dichalcogenide Semiconductors for 2D Optoelectronics. **2021**, e2107138   4

257   Artificial intelligence for search and discovery of quantum materials. **2021**, 2,   5

256   Electronic work function modulation of phosphorene by thermal oxidation. *2D Materials*,   5.9   1

255   Innovative Materials Science via Machine Learning. 2108044   9

254   Thermal Phase Control of Two-Dimensional Pt-Chalcogenide (Se and Te) Ultrathin Epitaxial Films and Nanocrystals. **2021**, 33, 8018-8027   0

253   Unified Treatment of Magnons and Excitons in Monolayer CrI_{3} from Many-Body Perturbation Theory. **2021**, 127, 166402   0

252   Screening and Understanding Li Adsorption on Two-Dimensional Metallic Materials by Learning Physics and Physics-Simplified Learning. **2021**, 1, 1904-1914   3

251	Computing Curie temperature of two-dimensional ferromagnets in the presence of exchange anisotropy. **2021**, 3,	3
250	Investigation of the thermoelectric properties of one-layer transition metal dichalcogenides. **2021**, 74, 270-278	2
249	Importance of Atomic-Like Basis Set Optimization for DFT Modelling of Nanomaterials. **2019**, 11, 44-50	0
248	Conclusions and Outlook. **2020**, 203-209	
247	Comprehensive search for buckled honeycomb binary compounds based on noble metals (Cu, Ag, and Au). **2021**, 5,	1
246	Robust recognition and exploratory analysis of crystal structures via Bayesian deep learning. **2021**, 12, 6234	3
245	ElTools: A tool for analyzing anisotropic elastic properties of the 2D and 3D materials. **2021**, 108195	4
244	Origin of phonon-limited mobility in two-dimensional metal dichalcogenides. **2021**, 34,	8
243	Time-Dependent Density Functional Theory Calculations of N- and S-Doped TiO Nanotube for Water-Splitting Applications. **2021**, 11,	2
242	Magnetism and Its Structural Coupling Effects in 2D Ising Ferromagnetic Insulator VI. **2021**, 21, 9180-9186	7
241	Accurate bandgap predictions of solids assisted by machine learning. **2021**, 29, 102932	1
240	Fundamentals of Graphene Plasmonics. **2020**, 71-100	
239	Analysis of Ionicity-Magnetism Competition in 2D-MX3 Halides towards a Low-Dimensional Materials Study Based on GPU-Enabled Computational Systems. **2021**, 11,	0
238	Janus monolayers of transition metal dichalcogenides a DFT study.	1
237	Strain-gated nonlinear Hall effect in two-dimensional MoSe2/WSe2 van der Waals heterostructure. **2021**, 104,	2
236	Tunable coupling of terahertz Dirac plasmons and phonons in transition metal dichalcogenide-based van der Waals heterostructures. *2D Materials*,	5.9
235	Novel 2D HfTeS4 for water splitting with high visible-light absorption. **2022**, 578, 151992	0
234	Generating stable molecules using imitation and reinforcement learning.	2

233   Scaling and Classification of Ion-Substrate Interaction.

| 232 | Honeycomb-like puckered PbSe with wide bandgap as promising thermoelectric material: a first-principles prediction. **2021**, 23, 100914 | 4 |

231   Research data infrastructure for high-throughput experimental materials science.. **2021**, 2, 100373   2

| 230 | Accelerated discovery of superoxide-dismutase nanozymes via high-throughput computational screening. **2021**, 12, 6866 | 12 |

229   Ab-initio investigation of Er3+ defects in tungsten disulfide. **2021**, 111041   0

| 228 | On-the-fly interpretable machine learning for rapid discovery of two-dimensional ferromagnets with high Curie temperature. **2021**, | 6 |

227   Long-term stability and tree-ring oxidation of WSe using phase-contrast AFM. **2021**, 13, 19238-19246   0

| 226 | On the Elastic Tensors of Ultra-Thin Films: A Study of Ruthenium. | |

225   Two-dimensional buckling structure induces the ultra-low thermal conductivity: a comparative study of the group GaX (X = N, P, As).   1

| 224 | Atomistic elucidation of mechanical properties and fracture phenomenon of defective indium selenide monolayer. **2022**, 30, e00637 | 0 |

223   High Throughput Investigation of an Emergent and Naturally Abundant 2D Material: Clinochlore.   0

| 222 | Antisite defect qubits in monolayer transition metal dichalcogenides.. **2022**, 13, 492 | 3 |

221   First-principles study of stability and electronic properties of single-element 2D materials. **2022**, 19, 92-98

| 220 | An study of two-dimensional anisotropic monolayers ScXY (X = S and Se; Y = Cl and Br) for photocatalytic water splitting applications with high carrier mobilities.. **2022**, | 1 |

219   Novel Two-Dimensional ABX Dirac Materials: Achieving a High-Speed Strain Sensor via a Self-Doping Effect.. **2022**, 13, 676-685   1

| 218 | Elastic properties of Janus transition metal dichalcogenide nanotubes from first principles. **2022**, 95, 1 | 0 |

217   Machine Learning Assisted Screening of Two-Dimensional Materials for Water Desalination.. **2022**,   1

| 216 | Length-Gauge Optical Matrix Elements in WIEN2k. **2022**, 10, 22 | 0 |

215	Machine learning assisted hierarchical filtering: a strategy for designing magnets with large moment and anisotropy energy.	0
214	Magnetism, symmetry and spin transport in van der Waals layered systems.	9
213	Autonomous Design of Photoferroic Ruddlesden-Popper Perovskites for Water Splitting Devices.. **2022**, 15,	1
212	MXene-based materials for remediation of environmental pollutants. **2022**, 553-594	
211	Universal co-existence of photovoltaics and ferroelectricity from a two-dimensional 3R bilayer BX (X = P, As, Sb). **2022**, 10, 1048-1061	0
210	Prospective on 2D Nanomaterials for Energy and Environment: Challenges, Commercial Aspect, and the Future Research Endeavor. **2022**, 267-329	0
209	Towards autonomous high-throughput multiscale modelling of battery interfaces.	3
208	Transition-metal nitride halide dielectrics for transition-metal dichalcogenide transistors.. **2021**, 14, 157-165	6
207	A bright future for engineering piezoelectric 2D crystals.. **2021**,	3
206	High-throughput assessment of two-dimensional electrode materials for energy storage devices. **2022**, 3, 100718	1
205	Electronic Structure of Monolayer FeSe on Si(001) from First Principles.. **2022**, 12,	
204	A machine learning model for screening thermodynamic stable lead-free halide double perovskites. **2022**, 204, 111172	4
203	Optical gaps and excitons in semiconducting transition metal carbides (MXenes).	2
202	Representing individual electronic states for machine learning GW band structures of 2D materials.. **2022**, 13, 468	4
201	Machine Learning Study of the Magnetic Ordering in 2D Materials.. **2022**,	2
200	Asymmetric XMoSiN2 (X=S, Se, Te) monolayers as novel promising 2D materials for nanoelectronics and photovoltaics. **2022**, 585, 152465	1
199	Workflow Engineering in Materials Design within the BATTERY 2030 + Project. 2102638	4
198	Relativistic Light Sails Need to Billow.. **2021**,	1

197	On the Contact of a Two-Dimensional Transition Metal with a Graphene-Like Compound. **2021**, 63, 796-801	
196	Functionalized few-layer silicene nanosheets: stability, elastic, structural, and electronic properties.. **2022**,	0
195	Understanding, discovery, and synthesis of 2D materials enabled by machine learning.. **2022**,	6
194	Designing light-element materials with large effective spin-orbit coupling.. **2022**, 13, 919	3
193	Graph-based discovery and analysis of atomic-scale one-dimensional materials.	1
192	Quantum theory of two-dimensional materials coupled to electromagnetic resonators. **2022**, 105,	1
191	Controllable Growth of ⊞and ⊟Antimonene by Interfacial Strain. **2022**, 126, 5022-5027	0
190	Efficient prediction of temperature-dependent elastic and mechanical properties of 2D materials.. **2022**, 12, 3776	1
189	Versatile band structure and electron⊟phonon coupling in layered PtSe2 with strong interlayer interaction. 1	1
188	Anisotropic Dzyaloshinskii-Moriya Interaction and Topological Magnetism in Two-Dimensional Magnets Protected by 4 2 Crystal Symmetry.. **2022**,	2
187	Autonomous high-throughput computations in catalysis. **2022**,	1
186	Strain engineering of Janus transition metal dichalcogenide nanotubes: an ab initio study. **2022**, 95, 1	0
185	Influence of Au, Ag, and Cu Adatoms on Optical Properties of TiO2 (110) Surface: Predictions from RT-TDDFT Calculations. **2022**, 12, 452	
184	A dataset of 175k stable and metastable materials calculated with the PBEsol and SCAN functionals.. **2022**, 9, 64	1
183	High-Throughput Computational Screening for Bipolar Magnetic Semiconductors.. **2022**, 2022, 9857631	0
182	Ab initio Screening of Two-dimensional CuQx and AgQx Chalcogenides.. **2022**,	
181	First principles design of 2 dimensional Nickel dichalcogenide Janus materials NiXY (X,Y´=´S,Se,Te). **2022**, 206, 111278	1
180	Quantum point defects in 2D materials - the QPOD database. **2022**, 8,	2

| 179 | On the elastic tensors of ultra-thin films: A study of ruthenium. **2022**, 153194 | 0 |

| 178 | Computational synthesis of 2D materials: A high-throughput approach to materials design. **2022**, 207, 111238 | 0 |

| 177 | Effect of a uniform random external magnetic field with spatiotemporal variation on compensation in Ising spin-1/2 trilayered square ferrimagnets.. **2021**, 104, 064126 | 0 |

| 176 | Theoretical study of stability, epitaxial formation, and phase transformations of two-dimensional pnictogen allotropes. **2021**, 104, | 0 |

| 175 | Elasticity-based-exfoliability measure for high-throughput computational exfoliation of two-dimensional materials. **2021**, 7, | 2 |

| 174 | First-principles study of electronic transport in germanane and hexagonal boron nitride. **2021**, 104, | 2 |

| 173 | Chemical hardness-driven interpretable machine learning approach for rapid search of photocatalysts. **2021**, 7, | 6 |

| 172 | Data-Driven Studies of the Magnetic Anisotropy of Two-Dimensional Magnetic Materials.. **2021**, 12, 12048-12054 | 14 |

| 171 | Oxygen Evolution and Reduction on Two-Dimensional Transition Metal Dichalcogenides.. **2021**, 58-65 | 6 |

| 170 | Efficient ionization of two-dimensional excitons by intense single-cycle terahertz pulses. **2021**, 104, | |

| 169 | Numerical quality control for DFT-based materials databases. **2022**, 8, | 1 |

| 168 | Rational Design of Heteroanionic Two-Dimensional Materials with Emerging Topological, Magnetic, and Dielectric Properties.. **2022**, 3594-3601 | 4 |

| 167 | Prediction of quantum anomalous Hall effect in CrI3/ScCl2 bilayer heterostructure. | |

| 166 | Data-Driven Approach to Designing Two-dimensional Van der Waals Heterostructures: Misjudgment of Band Alignment Type and its mechanism. | |

| 165 | Data_Sheet_1.PDF. **2020**, | |

| 164 | Data-Driven Materials Innovation and Applications.. **2022**, e2104113 | 2 |

| 163 | High-throughput inverse design and Bayesian optimization of functionalities: spin splitting in two-dimensional compounds.. **2022**, 9, 195 | |

| 162 | Scalable deeper graph neural networks for high-performance materials property prediction. **2022**, 3, 100491 | 2 |

161	Non-asymptotic quantum scattering theory to design high-mobility lateral transition-metal dichalcogenide heterostructures. **2022**, 131, 174302		0
160	Twist-resilient and robust ferroelectric quantum spin Hall insulators driven by van der Waals interactions. **2022**, 6,		0
159	High-Throughput Discovery and Investigation of Auxetic Two-Dimensional Crystals.		0
158	Exploring the structural and optoelectronic properties of natural insulating phlogopite in van der Waals heterostructures. *2D Materials*,	5.9	2
157	Gadolinium Halide Monolayers: A Fertile Family of Two-Dimensional 4f Magnets.		0
156	Computation-Aided Discovery and Synthesis of 2D PrOBr Photocatalyst. 1980-1986		0
155	Topological bands in PdSe2 pentagonal monolayer.		0
154	Prediction of 2D IV-VI semiconductors: auxetic materials with direct-gap and strong optical absorption.		1
153	Comprehensive understanding of intrinsic mobility and sub-10 nm quantum transportation in Ga2SSe monolayer.		3
152	Real- and momentum-space description of the excitons in bulk and monolayer chromium tri-halides. **2022**, 6,		1
151	Computational Discovery and Experimental Demonstration of Boron Phosphide Ultraviolet Nanoresonators. 2200422		3
150	Predicting Van der Waals Heterostructures by a Combined Machine Learning and Density Functional Theory Approach.		0
149	Accurate energy prediction of large-scale defective two-dimensional materials via deep learning. **2022**, 120, 213103		
148	High Thermoelectric Performance of Al2X2Se2 (X = Cl, Br, I) Monolayers with Strong Anisotropy in Lattice Thermal Conductivity.		2
147	Exciton binding energy and screening length in two-dimensional semiconductors. **2022**, 105,		0
146	Multilayer 2D insulator shows promise for post-silicon electronics. **2022**, 606, 37-38		
145	Novel boron nitride MXenes as promising energy storage materials.		0
144	2D Monolayers for Superior Transparent Electromagnetic Interference Shielding.		1

143	Toward machine learning for microscopic mechanisms: A formula search for crystal structure stability based on atomic properties. **2022**, 131, 215703		0
142	High-throughput computation and structure prototype analysis for two-dimensional ferromagnetic materials. **2022**, 8,		0
141	Growth of highly crystalline ultrathin two-dimensional selenene. *2D Materials*,	5.9	0
140	Boron-pnictogens: Highly anisotropic two-dimensional semiconductors for nanoelectronics and optoelectronics. **2022**, 6,		0
139	Plasmon-enhanced Raman spectroscopy of two-dimensional semiconductors. **2022**, 34, 333001		1
138	Inorganic Crystal Structure Prototype Database Based on Unsupervised Learning of Local Atomic Environments.		1
137	Two-dimensional host materials for lithium-sulfur batteries: A review and perspective. **2022**, 50, 696-717		1
136	High throughput investigation of an emergent and naturally abundant 2D material: Clinochlore. **2022**, 599, 153959		2
135	The rise of MAX phase alloys - large-scale theoretical screening for prediction of chemical order and disorder.		2
134	Lateral transition-metal dichalcogenide heterostructures for high efficiency thermoelectric devices.		2
133	Bandstructure and Transport Properties of Semiconducting Gallenene Nanoribbons. **2022**,		
132	Emergent Phenomena in Magnetic Two-Dimensional Materials and van der Waals Heterostructures.		2
131	Computational exfoliation of atomically thin one-dimensional materials with application to Majorana bound states. **2022**, 6,		0
130	Benchmarking exchange-correlation potentials with the mstar60 dataset: Importance of the nonlocal exchange potential for effective mass calculations in semiconductors. **2022**, 106,		0
129	Non-synchronous bulk photovoltaic effect in two-dimensional interlayer-sliding ferroelectrics. **2022**, 8,		1
128	A simple descriptor for magnetic classification of 2D MXene materials. **2022**, 12, 075106		
127	Toward Automated Computational Discovery of Battery Materials. 2200616		2
126	Machine-Learning-Assisted Acceleration on High-Symmetry Materials Search: Space Group Predictions from Band Structures.		0

125   Spin-orbital robust Dirac points in two-dimensional systems. **2022**, 27, 100774   0

124   Highly modulated dual semimetal and semiconducting ℇGeSe with strain engineering. *2D Materials*,   5.9   2

123   2D Material-Enabled Optical Rectennas with Ultrastrong Light-Electron Coupling. 2202199   0

122   Discovery of Two-Dimensional Multinary Component Photocatalysts Accelerated by Machine Learning. **2022**, 13, 7228-7235   1

121   Machine-Learning Assisted Exit-wave Reconstruction for Quantitative Feature Extraction. **2022**, 28, 2222-2224

120   Nonsymmorphic P21/m-MoTe 2 : Novel 2D Topological Materials. 2200188

119   Momentum-Dependent Oscillator Strength Crossover of Excitons and Plasmons in Two-Dimensional PtSe2. **2022**, 16, 12328-12337

118   Unravelling the regulating role of stacking pattern on the tunable dipole, mechanical behavior and carrier mobility for asymmetric Janus SnSSe bilayer. **2022**, 33, 104191

117   Polarization switching induced by domain wall sliding in two-dimensional ferroelectric monochalcogenides.   0

116   A theoretical roadmap for the best oxygen reduction activity in two-dimensional transition metal tellurides. **2022**, 13, 11048-11057   0

115   Anomalous dewetting growth of Si on Ag(111).   1

114   Geometry-modulated dipole polarizability of the two-dimensional Mott-Wannier excitons in gate-defined anisotropic quantum dot. **2022**, 12,   0

113   High-efficiency photocatalyst based on a MoSiGeN4/SiC heterojunction. **2022**, 57, 16404-16417   0

112   Excitonic instability in transition metal dichalcogenides. **2022**, 34, 455303   0

111   Resistive Switching Crossbar Arrays Based on Layered Materials. 2205402   2

110   Similarity of materials and data-quality assessment by fingerprinting.   0

109   Machine Learning-Aided Exploration of Ultrahard Materials. **2022**, 126, 15952-15961   0

108   Thermal Transport Properties of Na2X (X = O and S) Monolayers. **2022**, 12, 1294   0

| 107 | Recent Advancement in Rational Design Modulation of MXene: A Voyage from Environmental Remediation to Energy Conversion and Storage. | 1 |

| 106 | High-throughput design of functional-engineered MXene transistors with low-resistive contacts. **2022**, 8, | 5 |

| 105 | A universal similarity based approach for predictive uncertainty quantification in materials science. **2022**, 12, | 0 |

| 104 | Periodically Poled Monolayer Lithium Niobate for Photonic Chips of Quantum Devices. | 0 |

| 103 | Band alignment and interlayer hybridisation in transition metal dichalcogenide/hexagonal boron nitride heterostructures. | 0 |

| 102 | Chromium ditelluride monolayer: A novel promising 2H phase thermoelectric material with direct bandgap and ultralow lattice thermal conductivity. **2022**, 167485 | 1 |

| 101 | State-of-the-art progresses for Ti3C2Tx MXene reinforced polymer composites in corrosion and tribology aspects. **2022**, 309, 102790 | 0 |

| 100 | Exfoliation mechanisms of 2D materials and their applications. **2022**, 9, 041301 | 1 |

| 99 | Electronic and thermoelectric properties of semiconducting Bi2SSe2 and Bi2S2Se monolayers with high optical absorption. | 0 |

| 98 | Density-of-states similarity descriptor for unsupervised learning from materials data. **2022**, 9, | 1 |

| 97 | Two-dimensional heterostructures formed by graphenelike ZnO and MgO monolayers for optoelectronic applications. **2022**, 6, | 0 |

| 96 | Applications of MXene-Containing Polypyrrole Nanocomposites in Electrochemical Energy Storage and Conversion. | 2 |

| 95 | SnP2Se6: A Chiral 2D Semiconductor for High-Performance Electronics and Optoelectronics. | 0 |

| 94 | Machine-learning accelerated identification of exfoliable two-dimensional materials. | 0 |

| 93 | High-Throughput Characterization of Transition Metal Dichalcogenide Alloys: Thermodynamic Stability and Electronic Band Alignment. | 1 |

| 92 | M 3 C 2 (OH) 2 (M = Zr and Hf): An Ideal Electrode Material for sub-5 nm 2D Field-Effect Transistors. 2201166 | 0 |

| 91 | Photocatalytic activity of MoS2 with water monolayers: Global optimization. | 0 |

| 90 | Distinctive g-Factor of Moiré-Confined Excitons in van der Waals Heterostructures. | 2 |

89	Two-dimensional antiferromagnetic nodal-line semimetal and quantum anomalous Hall state in the van der Waals heterostructure germanene/Mn2S2. **2022**, 34, 505702	0
88	Abundance of Second Order Topology in C3 Symmetric Two-dimensional Insulators.	0
87	Recent Progress in Double-Layer Honeycomb Structure: A New Type of Two-Dimensional Material. **2022**, 15, 7715	1
86	Two-dimensional C3N/WS2 vdW heterojunction for direct Z-scheme photocatalytic overall water splitting. **2022**,	0
85	Toward Coarse-Grained Elasticity of Single-Layer Covalent Organic Frameworks.	0
84	Prediction of band gap of transition metal sulfide with Janus structure by deep learning atomic feature representation method. **2023**, 0	0
83	Prediction of electronic structure and magnetic anisotropy of two- dimensional MSi2N4 (M=3d transition-metal) monolayers. **2022**, 155693	0
82	Ferroelectric van der Waals heterostructures of CuInP2S6 for non-volatile memory device applications.	0
81	Machine Learning for Semiconductors. **2022**, 100033	0
80	Improving thermoelectric performance of asymmetrical Janus 1T-SnSSe monolayer by the synergistic effect of band convergence and crystal lattice softening under strain engineering. **2022**, 100923	1
79	Naturally-meaningful and efficient descriptors: machine learning of material properties based on robust one-shot ab initio descriptors. **2022**, 14,	1
78	Hole-doping induced ferromagnetism in 2D materials. **2022**, 8,	0
77	Investigation and understanding of the mechanical properties of MXene by high-throughput computations and interpretable machine learning. **2022**, 101921	0
76	Data-driven discovery of 2D materials by deep generative models. **2022**, 8,	0
75	Graphene multilayers for coherent perfectabsorption: effects of interlayer separation.	0
74	Reconstructing the exit wave of 2D materials in high-resolution transmission electron microscopy using machine learning. **2023**, 243, 113641	0
73	Graph neural networks for materials science and chemistry. **2022**, 3,	1
72	Perspective and Outlook. **2022**, 295-316	0

71	Designing two-dimensional ferroelectric materials from phosphorus-analogue structures.	0
70	Accurate property prediction with interpretable machine learning model for small datasets via transformed atom vector. **2022**, 6,	0
69	Device-System End-to-End Design of Photonic Neuromorphic Processor Using Reinforcement Learning. 2200381	0
68	On the bending of rectangular atomic monolayers along different directions: an ab initio study. **2023**, 34, 085701	0
67	WanTiBEXOS: a Wannier based Tight Binding code for electronic band structure, excitonic and optoelectronic properties of solids. **2022**, 108636	0
66	Capturing of non-hydrogenic Rydberg series of exciton binding energy in two-dimensional mono-layer WS2 using a modified Coulomb potential in fractional space. **2023**, 98, 015106	0
65	The Rise of Two-Dimensional-Material-Based Filters for Airborne Particulate Matter Removal.	1
64	Accurate prediction on the lattice thermal conductivities of monolayer systems by a high-throughput descriptor. **2023**, 56, 045304	0
63	Machine learning for membrane design and discovery. **2022**,	0
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61	High-Throughput Computational Screening of Two-Dimensional Semiconductors. **2022**, 13, 11581-11594	1
60	Predicting lattice thermal conductivity via machine learning: a mini review. **2023**, 9,	1
59	Benchmarking fundamental gap of Sc2C(OH)2 MXene by many-body methods.	0
58	Predicting the work function of 2D MXenes using machine-learning methods.	0
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56	Machine learning-based discovery of vibrationally stable materials. **2023**, 9,	0
55	Pressure-tuning the interlayer excitons in the GaS/HfS2 heterobilayer: A many-body perturbation simulation. **2023**, 614, 156272	0
54	Computational design of two-dimensional GeP based flexible strain sensor: Distinct J-V response. **2023**, 351, 114155	0

53   Novel metallic titanium fluoride: A promising high capacity and superionic conductivity anode in Li-, Na-, and K-ion batteries. **2023**, 210, 111822   0

52   Computational screening of two-dimensional substrates for stabilizing honeycomb borophene. **2023**, 615, 156388   0

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48   Hundreds of new, stable, one-dimensional materials from a generative machine learning model. **2023**, 7,   0

47   Trends in CO2 Reduction on Transition Metal Dichalcogenide Edges. 2341-2350   0

46   Predicting MXene Properties via Machine Learning. **2022**,   0

45   Solar cells based on 2D Janus group-III chalcogenide van der Waals heterostructures. **2023**, 15, 7126-7138   0

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43   General rules and applications for screening high phonon-limited mobility in two-dimensional semiconductors. **2023**, 107,   0

42   Structural and electronic properties of hexagonal MXH (M = C, Si, Ge and Sn; X = N, P, As and Sb) monolayers: A first-principles prediction. **2023**, 115710   0

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38   Thickness Determination of Ultrathin 2D Materials Empowered by Machine Learning Algorithms. **2023**, 17,   0

37   High-throughput computation of Raman spectra from first principles. **2023**, 10,   0

36   pyGWBSE: a high throughput workflow package for GW-BSE calculations. **2023**, 9,   0

35	Band Alignment of 2D Material Water Interfaces. **2023**, 127, 4132-4143	0
34	Antiferromagnetic topological magnetism in synthetic van der Waals antiferromagnets. **2023**, 107,	0
33	Theoretical Prediction of Semiconductor-Free Negative Differential Resistance Tunnel Diodes with High Peak-to-Valley Current Ratios Based on Two-Dimensional Cold Metals. **2023**, 6, 3758-3766	0
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27	AtomVision: A Machine Vision Library for Atomistic Images. **2023**, 63, 1708-1722	0
26	Hole doping induced ferromagnetism and Dzyaloshinskii Moriya interaction in the two-dimensional group-IVA oxides. **2023**, 35, 204003	0
25	Exploring and machine learning structural instabilities in 2D materials. **2023**, 9,	0
24	Shift current photovoltaic efficiency of 2D materials. **2023**, 9,	0
23	Thickness-dependent catalytic activity of hydrogen evolution based on single atomic catalyst of Pt above MXene. **2023**, 35, 204001	0
22	Connecting Higher-Order Topology with the Orbital Hall Effect in Monolayers of Transition Metal Dichalcogenides. **2023**, 130,	0
21	Unfolding the structure-property relationships of Li2S anchoring on two-dimensional materials with high-throughput calculations and machine learning. **2023**, 82, 31-39	0
20	Measuring complex refractive index through deep-learning-enabled optical reflectometry. **2023**, 10, 025025	0
19	Layer-dependent electronic structures and optical properties of two-dimensional PdSSe.	0
18	Investigating magnetic van der Waals materials using data-driven approaches.	0

17	Joining and arrangement of multilayers: A string representation for honeycomb layered materials. **2023**,	0
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15	Band-to-band tunneling switches based on two-dimensional van der Waals heterojunctions. **2023**, 10, 011318	0
14	Efficient GW calculations in two dimensional materials through a stochastic integration of the screened potential. **2023**, 9,	0
13	Infrared Photodetection from 2D/3D van der Waals Heterostructures. **2023**, 13, 1169	0
12	Two-dimensional ferroelectrics from high throughput computational screening. **2023**, 9,	0
11	HfXO (X = S and Se) Janus monolayers as promising two-dimensional platforms for optoelectronic and spintronic applications.	0
10	Descriptor engineering in machine learning regression of electronic structure properties for 2D materials. **2023**, 13,	0
9	Nonvolatile electrical control of spin polarization in the 2D bipolar magnetic semiconductor VSeF. **2023**, 9,	0
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6	High-Throughput First-Principles Prediction of Interfacial Adhesion Energies in Metal-on-Metal Contacts. **2023**, 15, 19624-19633	0
5	Accelerating the Discovery of Metastable IrO2 for the Oxygen Evolution Reaction by the Self-Learning-Input Graph Neural Network.	0
4	Artificial Intelligence Guided Studies of van der Waals Magnets.	0
3	MatHub-2d: A database for transport in 2D materials and a demonstration of high-throughput computational screening for high-mobility 2D semiconducting materials.	0
2	Mechanisms of Electronic and Ionic Transport during Mg Intercalation in MgS Cathode Materials and Their Decomposition Products.	0
1	High throughput calculations for a dataset of bilayer materials. **2023**, 10,	0