

Nabil Khossossi

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

320
papers

8,082
citations

45
h-index

77
g-index

340
ext. papers

9,985
ext. citations

5.4
avg, IF

6.71
L-index

| # | Paper | IF | Citations |
|-----|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|-----------|
| 320 | Binding and optical characteristics of polycyclic aromatic hydrocarbons and their nitroderivatives adsorbed on the C ₃ N monolayer. <i>New Journal of Chemistry</i> , 2022 , 46, 2245-2258 | 3.6 | 2 |
| 319 | Elucidating the reaction pathway of crystalline multi-metal borides for highly efficient oxygen-evolving electrocatalysts. <i>Journal of Materials Chemistry A</i> , 2022 , 10, 1569-1578 | 13 | 1 |
| 318 | Contact electrification through interfacial charge transfer: a mechanistic viewpoint on solid-liquid interfaces. <i>Nanoscale Advances</i> , 2022 , 4, 884-893 | 5.1 | 1 |
| 317 | Modified KBBF-like Material for Energy Storage Applications: ZnNiBO(OH) with Enhanced Cycle Life.. <i>ACS Applied Materials & Interfaces</i> , 2022 , | 9.5 | 5 |
| 316 | Exploring the relationship between Ln leaching and Ln-D binding energy in monazite (Nd, Sm, Eu). <i>Journal of the American Ceramic Society</i> , 2022 , 105, 553 | 3.8 | 1 |
| 315 | Preparation and properties of situ-sintered SiC ceramics aided by ZnO-Al ₂ O ₃ -CaO. <i>Journal of Alloys and Compounds</i> , 2022 , 890, 161854 | 5.7 | |
| 314 | Strain-mediated ferromagnetism and low-field magnetic reversal in Co doped monolayer [Formula: see text].. <i>Scientific Reports</i> , 2022 , 12, 2593 | 4.9 | 1 |
| 313 | Two-Dimensional Bismuthene Nanosheets for Selective Detection of Toxic Gases. <i>ACS Applied Nano Materials</i> , 2022 , 5, 2984-2993 | 5.6 | 2 |
| 312 | Strain modulating electronic band gaps and SQ efficiencies of semiconductor 2D PdQ (Q = S, Se) monolayer.. <i>Scientific Reports</i> , 2022 , 12, 2964 | 4.9 | 1 |
| 311 | Dynamical modeling of miR-34a, miR-449a, and miR-16 reveals numerous DDR signaling pathways regulating senescence, autophagy, and apoptosis in HeLa cells.. <i>Scientific Reports</i> , 2022 , 12, 4911 | 4.9 | 2 |
| 310 | Revealing the superlative electrochemical properties of o-B ₂ N ₂ monolayer in Lithium/Sodium-ion batteries. <i>Nano Energy</i> , 2022 , 96, 107066 | 17.1 | 6 |
| 309 | 2D Janus and non-Janus diamanes with an in-plane negative Poisson's ratio for energy applications. <i>Materials Today Advances</i> , 2022 , 14, 100225 | 7.4 | 1 |
| 308 | Janus Aluminum Oxysulfide Al ₂ OS: A promising 2D direct semiconductor photocatalyst with strong visible light harvesting. <i>Applied Surface Science</i> , 2022 , 589, 152997 | 6.7 | 3 |
| 307 | Antibodies Against Phosphorylcholine Among 60-Year-Olds: Clinical Role and Simulated Interactions.. <i>Frontiers in Cardiovascular Medicine</i> , 2022 , 9, 809007 | 5.4 | 1 |
| 306 | Stabilizing superconductivity of ternary metal pentahydride [Formula: see text] via electronic topological transitions under high pressure from first principles evolutionary algorithm.. <i>Scientific Reports</i> , 2022 , 12, 6700 | 4.9 | 0 |
| 305 | Bifunctional Catalytic Activity of 2D Boron Monochalcogenides BX (X = S, Se, Te). <i>Materials Today Energy</i> , 2022 , 101026 | 7 | 1 |
| 304 | Recent Advancements in Nontoxic Halide Perovskites: Beyond Divalent Composition Space.. <i>ACS Omega</i> , 2021 , 6, 33240-33252 | 3.9 | 0 |

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|-----|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----|----|
| 303 | Tuning the Nanoparticle Interfacial Properties and Stability of the Core-Shell Structure in Zn-Doped NiMoO@AWO. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 56116-56130 | 9.5 | 4 |
| 302 | Theoretical Prediction of a Bi-Doped Antimonene Monolayer as a Highly Efficient Photocatalyst for Oxygen Reduction and Overall Water Splitting. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 56234-56264 | 9.5 | 3 |
| 301 | Fabrication of BP2T functionalized graphene non-covalent π - π stacking interactions for enhanced ammonia detection.. <i>RSC Advances</i> , 2021 , 11, 35982-35987 | 3.7 | 1 |
| 300 | Pressure-induced order-disorder transitions in InS: an experimental and theoretical study of structural and vibrational properties. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 23625-23642 | 3.6 | 0 |
| 299 | Harnessing the unique properties of MXenes for advanced rechargeable batteries. <i>JPhys Energy</i> , 2021 , 3, 012005 | 4.9 | 7 |
| 298 | Mechanistic Understanding of the Interactions and Pseudocapacitance of Multi-Electron Redox Organic Molecules Sandwiched between MXene Layers. <i>Advanced Electronic Materials</i> , 2021 , 7, 2001202 | 6.4 | 1 |
| 297 | From Monolayers to Nanotubes: Toward Catalytic Transition-Metal Dichalcogenides for Hydrogen Evolution Reaction. <i>Energy & Fuels</i> , 2021 , 35, 6282-6288 | 4.1 | 2 |
| 296 | Salt-assisted growth of monolayer MoS2 for high-performance hysteresis-free field-effect transistor. <i>Journal of Applied Physics</i> , 2021 , 129, 145106 | 2.5 | 7 |
| 295 | Carbon Nitride Monolayers as Efficient Immobilizers toward Lithium Selenides: Potential Applications in Lithium Selenide Batteries. <i>ACS Applied Energy Materials</i> , 2021 , 4, 3891-3904 | 6.1 | 5 |
| 294 | Antimonene Allotropes β and γ Phases as Promising Anchoring Materials for Lithium Sulfur Batteries. <i>Energy & Fuels</i> , 2021 , 35, 9001-9009 | 4.1 | 4 |
| 293 | Lithium-functionalized boron phosphide nanotubes (BPNTs) as an efficient hydrogen storage carrier. <i>International Journal of Hydrogen Energy</i> , 2021 , 46, 20586-20593 | 6.7 | 7 |
| 292 | Degradation of Alzheimer's Amyloid- β by a Catalytically Inactive Insulin-Degrading Enzyme. <i>Journal of Molecular Biology</i> , 2021 , 433, 166993 | 6.5 | 7 |
| 291 | Modulation of 2D GaS/BTe vdW heterostructure as an efficient HER catalyst under external electric field influence. <i>Catalysis Today</i> , 2021 , 370, 14-25 | 5.3 | 5 |
| 290 | Ultrahigh carrier mobility and light-harvesting performance of 2D penta-PdX2 monolayer. <i>Journal of Materials Science</i> , 2021 , 56, 3846-3860 | 4.3 | 8 |
| 289 | Bain Deformation Mechanism and Lifshitz Transition in Magnesium under High Pressure. <i>Physica Status Solidi (B): Basic Research</i> , 2021 , 258, 2000279 | 1.3 | 6 |
| 288 | Mechanism of formaldehyde and formic acid formation on (101)-TiO2@Cu4 systems through CO2 hydrogenation. <i>Sustainable Energy and Fuels</i> , 2021 , 5, 564-574 | 5.8 | 1 |
| 287 | Thermodynamics and kinetics of 2D g-GeC monolayer as an anode materials for Li/Na-ion batteries. <i>Journal of Power Sources</i> , 2021 , 485, 229318 | 8.9 | 21 |
| 286 | Cs2InGaX6 (X=Cl, Br, or I): Emergent Inorganic Halide Double Perovskites with enhanced optoelectronic characteristics. <i>Current Applied Physics</i> , 2021 , 21, 50-57 | 2.6 | 13 |

285 No-Carbon 2D Anode Materials for Next-Generation Batteries **2021**, 1-14

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|-----|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----|----|
| 284 | Hydrogenation and oxidation enhances the thermoelectric performance of Si ₂ BN monolayer. <i>New Journal of Chemistry</i> , 2021 , 45, 3892-3900 | 3.6 | 0 |
| 283 | Pressure-promoted highly-ordered Fe-doped-Ni ₂ B for effective oxygen evolution reaction and overall water splitting. <i>Journal of Materials Chemistry A</i> , 2021 , 9, 6469-6475 | 13 | 10 |
| 282 | Data-Driven Machine Learning Approaches for Advanced Battery Modeling 2021 , 1-18 | | |
| 281 | Determining factors for the nano-biocompatibility of cobalt oxide nanoparticles: proximal discrepancy in intrinsic atomic interactions at differential vicinage. <i>Green Chemistry</i> , 2021 , 23, 3439-3458 ¹⁰ | | 11 |
| 280 | Formation of Lightweight Ternary Polyhydrides and Their Hydrogen Storage Mechanism. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 1723-1730 | 3.8 | 10 |
| 279 | MXene-Based 2D Anode Materials for Next-Generation Batteries 2021 , 1-20 | | |
| 278 | Design of Continuous Transport of the Droplet by the Contact-Boiling Regime. <i>Langmuir</i> , 2021 , 37, 553-560 | | 2 |
| 277 | Effect of Charge Injection on the Conducting Filament of Valence Change Anatase TiO Resistive Random Access Memory Device. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 1876-1884 | 6.4 | 7 |
| 276 | 8-16-4 graphyne: Square-lattice two-dimensional nodal line semimetal with a nontrivial topological Zak index. <i>Physical Review B</i> , 2021 , 103, | 3.3 | 8 |
| 275 | Stabilization and electronic topological transition of hydrogen-rich metal LiMoH under high pressures from first-principles predictions. <i>Scientific Reports</i> , 2021 , 11, 4079 | 4.9 | 6 |
| 274 | Large-Scale Fabrication of Wettability-Controllable Coatings for Optimizing Condensate Transfer Ability. <i>Langmuir</i> , 2021 , 37, 2476-2484 | 4 | 2 |
| 273 | Intrinsic atomic interaction at molecular proximal vicinity infer cellular biocompatibility of antibacterial nanopepper. <i>Nanomedicine</i> , 2021 , 16, 307-322 | 5.6 | 5 |
| 272 | Large-Scale Screening of Interface Parameters in the WC/W System Using Classical Force Field and First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 3631-3639 | 3.8 | 1 |
| 271 | Electronic and Transport Properties of Bilayer Phosphorene Nanojunction: Effect of Paired Substitution Doping. <i>ACS Applied Electronic Materials</i> , 2021 , 3, 733-742 | 4 | 5 |
| 270 | Understanding carbon dioxide capture on metal-organic frameworks from first-principles theory: The case of MIL-53(X), with X = Fe, Al, and Cu. <i>Journal of Chemical Physics</i> , 2021 , 155, 024701 | 3.9 | 1 |
| 269 | Role of atomicity in the oxygen reduction reaction activity of platinum sub nanometer clusters: A global optimization study. <i>Journal of Computational Chemistry</i> , 2021 , 42, 1944-1958 | 3.5 | 1 |
| 268 | Computational identification of efficient 2D Aluminium chalcogenides monolayers for optoelectronics and photocatalysts applications. <i>Applied Surface Science</i> , 2021 , 556, 149561 | 6.7 | 10 |

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|-----|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|----|
| 267 | High-Specific-Capacity and High-Performing Post-Lithium-Ion Battery Anode over 2D Black Arsenic Phosphorus. <i>ACS Applied Energy Materials</i> , 2021 , 4, 7900-7910 | 6.1 | 1 |
| 266 | High-temperature superconductor of sodalite-like clathrate hafnium hexahydride. <i>Scientific Reports</i> , 2021 , 11, 16403 | 4.9 | 2 |
| 265 | Correlation between reduced dielectric loss and charge migration kinetics in NdFeO ₃ -modified Ba _{0.7} Sr _{0.3} TiO ₃ ceramics. <i>Journal of Materials Science: Materials in Electronics</i> , 2021 , 32, 24910 | 2.1 | 0 |
| 264 | Coexisting commensurate and incommensurate charge ordered phases in CoO. <i>Scientific Reports</i> , 2021 , 11, 19415 | 4.9 | |
| 263 | Two-dimensional Janus Sn ₂ SSe and SnGeS ₂ semiconductors as strong absorber candidates for photovoltaic solar cells: First principles computations. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021 , 134, 114900 | 3 | 7 |
| 262 | Potential SiX (X = N, P, As, Sb, Bi) homo-bilayers for visible-light photocatalyst applications. <i>Catalysis Science and Technology</i> , 2021 , 11, 4996-5013 | 5.5 | 2 |
| 261 | Metallic one-dimensional heterostructure for gas molecule sensing. <i>Scientific Reports</i> , 2021 , 11, 433 | 4.9 | 0 |
| 260 | MXene binder stabilizes pseudocapacitance of conducting polymers. <i>Journal of Materials Chemistry A</i> , 2021 , 9, 20356-20361 | 13 | 1 |
| 259 | Local electrocatalytic activity of PtRu supported on nitrogen-doped carbon nanotubes towards methanol oxidation by scanning electrochemical microscopy. <i>Journal of Materials Chemistry A</i> , 2021 , 9, 21291-21301 | 13 | 3 |
| 258 | Highly Sensitive Gas Sensing Material for Environmentally Toxic Gases Based on Janus NbSeTe Monolayer. <i>Nanomaterials</i> , 2020 , 10, | 5.4 | 5 |
| 257 | Poisonous Vapor Adsorption on Pure and Modified Aluminum Nitride Nanosheet for Environmental Safety: A DFT Exploration. <i>Sustainability</i> , 2020 , 12, 10097 | 3.6 | |
| 256 | Highly Energetic and Stable Gadolinium/Bismuth Molybdate with a Fast Reactive Species, Redox Mechanism of Aqueous Electrolyte. <i>ACS Applied Energy Materials</i> , 2020 , 3, 12385-12399 | 6.1 | 6 |
| 255 | Mechanical and electronic properties of van der Waals layered hcp PdH. <i>Scientific Reports</i> , 2020 , 10, 8037 | 4.9 | 1 |
| 254 | Molecules versus Nanoparticles: Identifying a Reactive Molecular Intermediate in the Synthesis of Ternary Coinage Metal Chalcogenides. <i>Inorganic Chemistry</i> , 2020 , 59, 7727-7738 | 5.1 | 8 |
| 253 | Metal-functionalized 2D boron sulfide monolayer material enhancing hydrogen storage capacities. <i>Journal of Applied Physics</i> , 2020 , 127, 184305 | 2.5 | 9 |
| 252 | Structural Phase Transitions, Electronic Properties, and Hardness of RuB ₄ under High Pressure in Comparison with FeB ₄ and OsB ₄ . <i>Journal of Physical Chemistry C</i> , 2020 , 124, 14804-14810 | 3.8 | 10 |
| 251 | Hydrogen storage characteristics of Li and Na decorated 2D boron phosphide. <i>Sustainable Energy and Fuels</i> , 2020 , 4, 4538-4546 | 5.8 | 21 |
| 250 | Structure-based drug designing and immunoinformatics approach for SARS-CoV-2. <i>Science Advances</i> , 2020 , 6, eabb8097 | 14.3 | 97 |

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|-----|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|----|
| 249 | Exploring the Possibility of EPhase Arsenic-Phosphorus Polymorph Monolayer as Anode Materials for Sodium-Ion Batteries. <i>Advanced Theory and Simulations</i> , 2020 , 3, 2000023 | 3.5 | 8 |
| 248 | Effect of Cycling Ion and Solvent on the Redox Chemistry of Substituted Quinones and Solvent-Induced Breakdown of the Correlation between Redox Potential and Electron-Withdrawing Power of Substituents. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 13609-13617 | 3.8 | 12 |
| 247 | Enhancement of hydrogen storage capacity on co-functionalized GaS monolayer under external electric field. <i>International Journal of Hydrogen Energy</i> , 2020 , 45, 12384-12393 | 6.7 | 12 |
| 246 | Strain-Engineered Metal-Free h-B2O Monolayer as a Mechanocatalyst for Photocatalysis and Improved Hydrogen Evolution Reaction. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 7884-7892 | 3.8 | 9 |
| 245 | Carbides-anti-perovskites Mn ₃ (Sn, Zn)C: Potential candidates for an application in magnetic refrigeration. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020 , 124, 114317 | 3 | 2 |
| 244 | 2D monolayer boron sulfide as an efficient material for optical nanodevices 2020 , | | 1 |
| 243 | Capacity enhancement of polyolithiated functionalized boron nitride nanotubes: an efficient hydrogen storage medium. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 15675-15682 | 3.6 | 5 |
| 242 | Van der Waals induced molecular recognition of canonical DNA nucleobases on a 2D GaS monolayer. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 6706-6715 | 3.6 | 4 |
| 241 | Two-dimensional boron monochalcogenide monolayer for thermoelectric material. <i>Sustainable Energy and Fuels</i> , 2020 , 4, 2363-2369 | 5.8 | 37 |
| 240 | Rectifying behavior in twisted bilayer black phosphorus nanojunctions mediated through intrinsic anisotropy. <i>Nanoscale Advances</i> , 2020 , 2, 1493-1501 | 5.1 | 9 |
| 239 | Room-temperature conversion of CuSe to CuAgSe nanoparticles to enhance the photocatalytic performance of their composites with TiO ₂ . <i>Dalton Transactions</i> , 2020 , 49, 3580-3591 | 4.3 | 9 |
| 238 | Exploring two-dimensional M ₂ NS ₂ (M = Ti, V) MXenes based gas sensors for air pollutants. <i>Applied Materials Today</i> , 2020 , 19, 100574 | 6.6 | 20 |
| 237 | HfS ₂ and TiS ₂ Monolayers with Adsorbed C, N, P Atoms: A First Principles Study. <i>Catalysts</i> , 2020 , 10, 94 | 4 | 1 |
| 236 | Necklace-like Nitrogen-Doped Tubular Carbon 3D Frameworks for Electrochemical Energy Storage. <i>Advanced Functional Materials</i> , 2020 , 30, 1909725 | 15.6 | 46 |
| 235 | Superior sensitivity of metal functionalized boron carbide (BC ₃) monolayer towards carbonaceous pollutants. <i>Applied Surface Science</i> , 2020 , 512, 145637 | 6.7 | 9 |
| 234 | Crystallography of low Z material at ultrahigh pressure: Case study on solid hydrogen. <i>Matter and Radiation at Extremes</i> , 2020 , 5, 038401 | 4.7 | 11 |
| 233 | Unraveling the single-atom electrocatalytic activity of transition metal-doped phosphorene. <i>Nanoscale Advances</i> , 2020 , 2, 2410-2421 | 5.1 | 5 |
| 232 | Interplay of charge density wave and multiband superconductivity in layered quasi-two-dimensional materials: The case of 2H _{1-x} NbS ₂ and 2H _{1-x} NbSe ₂ . <i>Physical Review Materials</i> , 2020 , 4, | 3.2 | 15 |

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| 231 | Carbon-phosphide monolayer with high carrier mobility and perceptible I _V response for superior gas sensing. <i>New Journal of Chemistry</i> , 2020 , 44, 3777-3785 | 3.6 | 15 |
| 230 | Progress in supercapacitors: roles of two dimensional nanotubular materials. <i>Nanoscale Advances</i> , 2020 , 2, 70-108 | 5.1 | 91 |
| 229 | Li-decorated carbyne for hydrogen storage: charge induced polarization and van't Hoff hydrogen desorption temperature. <i>Sustainable Energy and Fuels</i> , 2020 , 4, 691-699 | 5.8 | 8 |
| 228 | Remarkable improvement in hydrogen storage capacities of two-dimensional carbon nitride (g-C ₃ N ₄) nanosheets under selected transition metal doping. <i>International Journal of Hydrogen Energy</i> , 2020 , 45, 3035-3045 | 6.7 | 43 |
| 227 | Terahertz plasmonics: The rise of toroidal metadvice towards immunobiosensings. <i>Materials Today</i> , 2020 , 32, 108-130 | 21.8 | 148 |
| 226 | Recent Advancements and Future Prospects in Ultrathin 2D Semiconductor-Based Photocatalysts for Water Splitting. <i>Catalysts</i> , 2020 , 10, 1111 | 4 | 18 |
| 225 | Exploring the Degradation Behavior of Ce-Monazite in Water Solution through Adsorption and Penetration Kinetics. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 22173-22184 | 3.8 | 5 |
| 224 | Tuning Hydrogen Storage Properties of Carbon Nanosheets through Selected Foreign Metal Functionalization. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 16827-16837 | 3.8 | 5 |
| 223 | Rational Design of 2D h-BAs Monolayer as Advanced Sulfur Host for High Energy Density LiS Batteries. <i>ACS Applied Energy Materials</i> , 2020 , 3, 7306-7317 | 6.1 | 10 |
| 222 | Core-shell nanostructures: perspectives towards drug delivery applications. <i>Journal of Materials Chemistry B</i> , 2020 , | 7.3 | 61 |
| 221 | Emerging piezochromism in transparent lead free perovskite Rb ₃ X ₂ I ₉ (X = Sb, Bi) under compression: A comparative theoretical insight. <i>Journal of Applied Physics</i> , 2020 , 128, 045102 | 2.5 | 2 |
| 220 | Ultrathin nanowire PdX ₂ (X = P, As): stability, electronic transport and thermoelectric properties. <i>New Journal of Chemistry</i> , 2020 , 44, 15617-15624 | 3.6 | 0 |
| 219 | Emerging piezochromism in lead free alkaline earth chalcogenide perovskite AZrS ₃ (A = Mg, Ca, Sr and Ba) under pressure. <i>Journal of Materials Chemistry C</i> , 2020 , 8, 16392-16403 | 7.1 | 9 |
| 218 | Route to high-[Formula: see text] superconductivity of [Formula: see text] via strong bonding of boron-carbon compound at high pressure. <i>Scientific Reports</i> , 2020 , 10, 18090 | 4.9 | 9 |
| 217 | Structural Insight of the Frailty of 2D Janus NbSeTe as an Active Photocatalyst. <i>ChemCatChem</i> , 2020 , 12, 6013-6023 | 5.2 | 12 |
| 216 | Temperature-Dependent Cationic Doping-Driven Phonon Dynamics Investigation in CdO Thin Films Using Raman Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 21818-21828 | 3.8 | 3 |
| 215 | Toroidal Metaphotonics and Metadvice. <i>Laser and Photonics Reviews</i> , 2020 , 14, 1900326 | 8.3 | 51 |
| 214 | Zn Metal Atom Doping on the Surface Plane of One-Dimensional NiMoO Nanorods with Improved Redox Chemistry. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 44815-44829 | 9.5 | 26 |

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| 213 | Optical excitations and thermoelectric properties of two-dimensional holey graphene. <i>Physical Review B</i> , 2020 , 102, | 3.3 | 12 |
| 212 | Recent progress of defect chemistry on 2D materials for advanced battery anodes. <i>Chemistry - an Asian Journal</i> , 2020 , 15, 3390-3404 | 4.5 | 15 |
| 211 | Density Functional Theory Studies of Si ₂ BN Nanosheets as Anode Materials for Magnesium-Ion Batteries. <i>ACS Applied Nano Materials</i> , 2020 , 3, 9055-9063 | 5.6 | 11 |
| 210 | Ultralow Thermal Conductivity and High Thermoelectric Figure of Merit in Two-Dimensional Thallium Selenide. <i>ACS Applied Energy Materials</i> , 2020 , 3, 9315-9325 | 6.1 | 7 |
| 209 | Elucidating hydrogen storage properties of two-dimensional siligraphene (SiC ₈) monolayers upon selected metal decoration. <i>Sustainable Energy and Fuels</i> , 2020 , 4, 5578-5587 | 5.8 | 10 |
| 208 | High Thermoelectric Performance in Two-Dimensional Janus Monolayer Material WS-X (= Se and Te). <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 46212-46219 | 9.5 | 35 |
| 207 | Impact of edge structures on interfacial interactions and efficient visible-light photocatalytic activity of metal-semiconductor hybrid 2D materials. <i>Catalysis Science and Technology</i> , 2020 , 10, 3279-3289 | 5.5 | 24 |
| 206 | Sensing the polar molecules MH ₃ (M = N, P, or As) with a Janus NbTeSe monolayer. <i>New Journal of Chemistry</i> , 2020 , 44, 7932-7940 | 3.6 | 15 |
| 205 | Cesium Bismuth Iodide Solar Cells from Systematic Molar Ratio Variation of CsI and BiI ₃ . <i>Inorganic Chemistry</i> , 2019 , 58, 12040-12052 | 5.1 | 23 |
| 204 | An emerging Janus MoSeTe material for potential applications in optoelectronic devices. <i>Journal of Materials Chemistry C</i> , 2019 , 7, 12312-12320 | 7.1 | 45 |
| 203 | Ab Initio Screening of Doped Mg(AlH) Systems for Conversion-Type Lithium Storage. <i>Materials</i> , 2019 , 12, | 3.5 | 4 |
| 202 | Elemental Substitution of Two-Dimensional Transition Metal Dichalcogenides (MoSe and MoTe): Implications for Enhanced Gas Sensing. <i>ACS Sensors</i> , 2019 , 4, 2646-2653 | 9.2 | 42 |
| 201 | Structural Evolution of AlN Nanoclusters and the Elemental Chemisorption Characteristics: Atomistic Insight. <i>Nanomaterials</i> , 2019 , 9, | 5.4 | 1 |
| 200 | Phase evolution in calcium molybdate nanoparticles as a function of synthesis temperature and its electrochemical effect on energy storage. <i>Nanoscale Advances</i> , 2019 , 1, 565-580 | 5.1 | 24 |
| 199 | Mapping the sodium intercalation mechanism, electrochemical properties and structural evolution in non-stoichiometric alluaudite Na _{2+2x} Fe ₂ (SO ₄) ₃ cathode materials. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 17446-17455 | 13 | 4 |
| 198 | Hybrid-Functional Study of Native Defects and W/Mo-Doped in Monoclinic-Bismuth Vanadate. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 14508-14516 | 3.8 | 5 |
| 197 | Li-Functionalized Carbon Nanotubes for Hydrogen Storage: Importance of Size Effects. <i>ACS Applied Nano Materials</i> , 2019 , 2, 3021-3030 | 5.6 | 15 |
| 196 | Ground-state structure of semiconducting and superconducting phases in xenon carbides at high pressure. <i>Scientific Reports</i> , 2019 , 9, 2459 | 4.9 | 13 |

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|-----|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|----|
| 195 | Aero-gel based CeO ₂ nanoparticles: synthesis, structural properties and detailed humidity sensing response. <i>Journal of Materials Chemistry C</i> , 2019 , 7, 5477-5487 | 7.1 | 44 |
| 194 | Enhanced Optoelectronic and Thermoelectric Properties by Intrinsic Structural Defects in Monolayer HfS ₂ . <i>ACS Applied Energy Materials</i> , 2019 , 2, 6891-6903 | 6.1 | 17 |
| 193 | Probing the active sites of newly predicted stable Janus scandium dichalcogenides for photocatalytic water-splitting. <i>Catalysis Science and Technology</i> , 2019 , 9, 4981-4989 | 5.5 | 20 |
| 192 | Inquisitive Geometric Sites in h-BN Monolayer for Alkali Earth Metal Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 19340-19346 | 3.8 | 8 |
| 191 | Ab initio study of a 2D h-BAs monolayer: a promising anode material for alkali-metal ion batteries. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 18328-18337 | 3.6 | 26 |
| 190 | Defect Thermodynamics in Nonstoichiometric Alluaudite-Based Polyanionic Materials for Na-Ion Batteries. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 32856-32868 | 9.5 | 2 |
| 189 | Interfacial aspect of ZnTe/In ₂ Te ₃ heterostructures as an efficient catalyst for the hydrogen evolution reaction. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 27441-27449 | 13 | 27 |
| 188 | Investigation of the Factors That Dictate the Preferred Orientation of Lexitropsins in the Minor Groove of DNA. <i>Journal of Medicinal Chemistry</i> , 2019 , 62, 10423-10440 | 8.3 | 3 |
| 187 | Modelling high-performing batteries with Mxenes: The case of S-functionalized two-dimensional nitride Mxene electrode. <i>Nano Energy</i> , 2019 , 58, 877-885 | 17.1 | 62 |
| 186 | The influence of edge structure on the optoelectronic properties of Si ₂ BN quantum dot. <i>Journal of Applied Physics</i> , 2019 , 126, 233104 | 2.5 | 7 |
| 185 | Effect of electric field on optoelectronic properties of indiene monolayer for photoelectric nanodevices. <i>Scientific Reports</i> , 2019 , 9, 17300 | 4.9 | 9 |
| 184 | Emergence of Si ₂ BN Monolayer as Efficient HER Catalyst under Co-functionalization Influence. <i>ACS Applied Energy Materials</i> , 2019 , 2, 8441-8448 | 6.1 | 9 |
| 183 | Ultrahigh-pressure isostructural electronic transitions in hydrogen. <i>Nature</i> , 2019 , 573, 558-562 | 50.4 | 47 |
| 182 | Dynamic magneto-caloric effect of a multilayer nanographene: Dynamic quantum Monte Carlo. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2019 , 105, 139-145 | 3 | 12 |
| 181 | TiS Monolayer as an Emerging Ultrathin Bifunctional Catalyst: Influence of Defects and Functionalization. <i>ChemPhysChem</i> , 2019 , 20, 608-617 | 3.2 | 14 |
| 180 | Theoretical investigation of the structural, electronic, and thermodynamic properties of CdS _{1-x} Sex alloys. <i>Journal of Applied Physics</i> , 2018 , 123, 105103 | 2.5 | 5 |
| 179 | 2D lateral heterostructures of group-III monochalcogenide: Potential photovoltaic applications. <i>Applied Physics Letters</i> , 2018 , 112, 143902 | 3.4 | 43 |
| 178 | Structural prediction of host-guest structure in lithium at high pressure. <i>Scientific Reports</i> , 2018 , 8, 52784.9 | 17 | |

| | | | |
|-----|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----|----|
| 177 | Chemical Bonding of Unique CO on Fe(100). <i>Journal of Physical Chemistry C</i> , 2018 , 122, 9062-9074 | 3.8 | 1 |
| 176 | The High-Pressure Superconducting Phase of Arsenic. <i>Scientific Reports</i> , 2018 , 8, 3026 | 4.9 | 9 |
| 175 | Theoretical aspects in structural distortion and the electronic properties of lithium peroxide under high pressure. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 9488-9497 | 3.6 | 2 |
| 174 | Alloying in an Intercalation Host: Metal Titanium Niobates as Anodes for Rechargeable Alkali-Ion Batteries. <i>Chemistry - an Asian Journal</i> , 2018 , 13, 299-310 | 4.5 | 3 |
| 173 | Metallized siligraphene nanosheets (SiC7) as high capacity hydrogen storage materials. <i>Nano Research</i> , 2018 , 11, 3802-3813 | 10 | 37 |
| 172 | Defected and Functionalized Germanene-based Nanosensors under Sulfur Comprising Gas Exposure. <i>ACS Sensors</i> , 2018 , 3, 867-874 | 9.2 | 33 |
| 171 | Theoretical Evidence behind Bifunctional Catalytic Activity in Pristine and Functionalized Al C Monolayers. <i>ChemPhysChem</i> , 2018 , 19, 148-152 | 3.2 | 8 |
| 170 | Borophene's tryst with stability: exploring 2D hydrogen boride as an electrode for rechargeable batteries. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 22008-22016 | 3.6 | 31 |
| 169 | Scrupulous Probing of Bifunctional Catalytic Activity of Borophene Monolayer: Mapping Reaction Coordinate with Charge Transfer. <i>ACS Applied Energy Materials</i> , 2018 , 1, 3571-3576 | 6.1 | 26 |
| 168 | Achieving ultrahigh carrier mobilities and opening the band gap in two-dimensional SiBN. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 21716-21723 | 3.6 | 18 |
| 167 | Simultaneous enhancement in charge separation and onset potential for water oxidation in a BiVO ₄ photoanode by W ^{VI} codoping. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 16965-16974 | 13 | 22 |
| 166 | Tuning electronic transport properties of zigzag graphene nanoribbons with silicon doping and phosphorus passivation. <i>AIP Advances</i> , 2018 , 8, 085123 | 1.5 | 8 |
| 165 | New Concept on Photocatalytic Degradation of Thiophene Derivatives: Experimental and DFT Studies. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 15646-15651 | 3.8 | 4 |
| 164 | Theoretical Investigation of Metallic Nanolayers For Charge-Storage Applications. <i>ACS Applied Energy Materials</i> , 2018 , 1, 3428-3433 | 6.1 | 15 |
| 163 | Efficient Adsorption Characteristics of Pristine and Silver-Doped Graphene Oxide Towards Contaminants: A Potential Membrane Material for Water Purification?. <i>ChemPhysChem</i> , 2018 , 19, 2250-2257 | 3.2 | 10 |
| 162 | The ideal commensurate value of Sc and the superconducting phase under high pressure. <i>Journal of Applied Physics</i> , 2018 , 124, 225901 | 2.5 | 15 |
| 161 | Hexagonal Boron Nitride (h-BN) Sheets Decorated with OLi, ONa, and Li F Molecules for Enhanced Energy Storage. <i>ChemPhysChem</i> , 2017 , 18, 513-518 | 3.2 | 30 |
| 160 | A comparative study of hydrogen evolution reaction on pseudo-monolayer WS ₂ and PtS ₂ : insights based on the density functional theory. <i>Catalysis Science and Technology</i> , 2017 , 7, 687-692 | 5.5 | 42 |

| | | | |
|-----|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|-----|
| 159 | Designing strategies to tune reduction potential of organic molecules for sustainable high capacity battery application. <i>Journal of Materials Chemistry A</i> , 2017 , 5, 4430-4454 | 13 | 41 |
| 158 | Role of relativity in high-pressure phase transitions of thallium. <i>Scientific Reports</i> , 2017 , 7, 42983 | 4.9 | 3 |
| 157 | Rational Design: A High-Throughput Computational Screening and Experimental Validation Methodology for Lead-Free and Emergent Hybrid Perovskites. <i>ACS Energy Letters</i> , 2017 , 2, 837-845 | 20.1 | 142 |
| 156 | Unsaturated surface in CO saturation. <i>Surface and Interface Analysis</i> , 2017 , 49, 892-897 | 1.5 | 2 |
| 155 | Effect of Transition Metal Cations on Stability Enhancement for Molybdate-Based Hybrid Supercapacitor. <i>ACS Applied Materials & Interfaces</i> , 2017 , 9, 17977-17991 | 9.5 | 61 |
| 154 | Enabling the Electrochemical Activity in Sodium Iron Metaphosphate [NaFe(PO)] Sodium Battery Insertion Material: Structural and Electrochemical Insights. <i>Inorganic Chemistry</i> , 2017 , 56, 5918-5929 | 5.1 | 24 |
| 153 | Borophane as a Benchmark of Graphene: A Potential 2D Material for Anode of Li and Na-Ion Batteries. <i>ACS Applied Materials & Interfaces</i> , 2017 , 9, 16148-16158 | 9.5 | 101 |
| 152 | Magnetic order and phase diagram of magnetic alloy system: Mg _x Ni _{1-x} O alloy. <i>Physica Status Solidi (B): Basic Research</i> , 2017 , 254, 1700085 | 1.3 | 3 |
| 151 | Anisotropic distortion and Lifshitz transition in Hf under pressure. <i>Physical Review B</i> , 2017 , 95, | 3.3 | 8 |
| 150 | Stability of Ar(H) to 358 GPa. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017 , 114, 3596-3600 | 11.5 | 16 |
| 149 | Assessing the electrochemical properties of polypyridine and polythiophene for prospective applications in sustainable organic batteries. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 3307-3314 | 3.6 | 12 |
| 148 | Sensitive and selective detection of copper ions using low cost nitrogen doped carbon quantum dots as a fluorescent sensing platform. <i>ISSS Journal of Micro and Smart Systems</i> , 2017 , 6, 109-117 | 0.9 | 13 |
| 147 | Mechanistic study of Na-ion diffusion and small polaron formation in K ₂ Fe(SO ₄) ₂ ·2H ₂ O based cathode materials. <i>Journal of Materials Chemistry A</i> , 2017 , 5, 21726-21739 | 13 | 15 |
| 146 | The curious case of two dimensional Si ₂ BN: A high-capacity battery anode material. <i>Nano Energy</i> , 2017 , 41, 251-260 | 17.1 | 68 |
| 145 | Bromination-induced stability enhancement with a multivalley optical response signature in guanidinium [C(NH ₂) ₃] ⁺ -based hybrid perovskite solar cells. <i>Journal of Materials Chemistry A</i> , 2017 , 5, 18561-18568 | 13 | 8 |
| 144 | High performance material for hydrogen storage: Graphenelike Si ₂ BN solid. <i>International Journal of Hydrogen Energy</i> , 2017 , 42, 22942-22952 | 6.7 | 33 |
| 143 | Toward the Realization of 2D Borophene Based Gas Sensor. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 26869-26876 | 3.8 | 98 |
| 142 | Prospects of Graphene-hBN Heterostructure Nanogap for DNA Sequencing. <i>ACS Applied Materials & Interfaces</i> , 2017 , 9, 39945-39952 | 9.5 | 29 |

| | | | |
|-----|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|-----|
| 141 | Divulging the Hidden Capacity and Sodiation Kinetics of $\text{Na}_x\text{C}_6\text{Cl}_4\text{O}_2$: A High Voltage Organic Cathode for Sodium Rechargeable Batteries. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 14027-14036 | 3.8 | 12 |
| 140 | Formation and electronic properties of palladium hydrides and palladium-rhodium dihydride alloys under pressure. <i>Scientific Reports</i> , 2017 , 7, 3520 | 4.9 | 13 |
| 139 | Studies of hypro-mellose (HPMC) functionalized ZnS:Mn fluorescent quantum dots. <i>Journal of Materials Science: Materials in Electronics</i> , 2017 , 28, 1931-1937 | 2.1 | 3 |
| 138 | Review of two-dimensional materials for photocatalytic water splitting from a theoretical perspective. <i>Catalysis Science and Technology</i> , 2017 , 7, 545-559 | 5.5 | 251 |
| 137 | Sensing Characteristics of Phosphorene Monolayers toward PH_3 and AsH_3 Gases upon the Introduction of Vacancy Defects. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 20428-20436 | 3.8 | 52 |
| 136 | Time dependent DFT investigation of the optical response in pristine and Gd doped Al_2O_3 . <i>RSC Advances</i> , 2016 , 6, 72537-72543 | 3.7 | 1 |
| 135 | Probing the pseudo-1-D ion diffusion in lithium titanium niobate anode for Li-ion battery. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 22323-30 | 3.6 | 14 |
| 134 | Defect and Substitution-Induced Silicene Sensor to Probe Toxic Gases. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 25256-25262 | 3.8 | 63 |
| 133 | 2D-HfS ₂ as an efficient photocatalyst for water splitting. <i>Catalysis Science and Technology</i> , 2016 , 6, 6605-6614 | 5.14 | 52 |
| 132 | Density Functional Theory Study of Hydrogen Adsorption in a Ti-Decorated Mg-Based Metal-Organic Framework-74. <i>ChemPhysChem</i> , 2016 , 17, 879-84 | 3.2 | 15 |
| 131 | Evaluating bulk $\text{Nb}_2\text{O}_2\text{F}_3$ for Li-battery electrode applications. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 3530-5 | 3.6 | |
| 130 | Rationalizing the Hydrogen and Oxygen Evolution Reaction Activity of Two-Dimensional Hydrogenated Silicene and Germanene. <i>ACS Applied Materials & Interfaces</i> , 2016 , 8, 1536-44 | 9.5 | 56 |
| 129 | $\text{NaCo}(\text{SO})$ as a new member of the alluaudite family of high-voltage sodium battery cathodes. <i>Dalton Transactions</i> , 2016 , 46, 55-63 | 4.3 | 39 |
| 128 | Two-dimensional boron: Lightest catalyst for hydrogen and oxygen evolution reaction. <i>Applied Physics Letters</i> , 2016 , 109, 053903 | 3.4 | 71 |
| 127 | Rare earth functionalization effect in optical response of ZnO nano clusters. <i>European Physical Journal D</i> , 2016 , 70, 1 | 1.3 | 4 |
| 126 | Ionothermal Synthesis of High-Voltage Alluaudite $\text{Na}_{2+2x}\text{Fe}_{2-x}(\text{SO}_4)_3$ Sodium Insertion Compound: Structural, Electronic, and Magnetic Insights. <i>ACS Applied Materials & Interfaces</i> , 2016 , 8, 6982-91 | 9.5 | 52 |
| 125 | Unveiling the thermodynamic and kinetic properties of $\text{Na}_x\text{Fe}(\text{SO}_4)_2$ ($x = 0\bar{2}$): toward a high-capacity and low-cost cathode material. <i>Journal of Materials Chemistry A</i> , 2016 , 4, 17960-17969 | 13 | 12 |
| 124 | High pressure-induced distortion in face-centered cubic phase of thallium. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016 , 113, 11143-11147 | 11.5 | 8 |

| | | | |
|-----|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|-----|
| 123 | Establishing the most favorable metal-carbon bond strength for carbon nanotube catalysts. <i>Journal of Materials Chemistry C</i> , 2015 , 3, 3422-3427 | 7.1 | 24 |
| 122 | Na _{2.44} Mn _{1.79} (SO ₄) ₃ : a new member of the alluaudite family of insertion compounds for sodium ion batteries. <i>Journal of Materials Chemistry A</i> , 2015 , 3, 18564-18571 | 13 | 82 |
| 121 | Defect Engineered g-C ₃ N ₄ for Efficient Visible Light Photocatalytic Hydrogen Production. <i>Chemistry of Materials</i> , 2015 , 27, 4930-4933 | 9.6 | 308 |
| 120 | Highly Sensitive and Selective Gas Detection Based on Silicene. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 16934-16940 | 3.8 | 131 |
| 119 | Synthesis, and crystal and electronic structure of sodium metal phosphate for use as a hybrid capacitor in non-aqueous electrolyte. <i>Dalton Transactions</i> , 2015 , 44, 20108-20 | 4.3 | 38 |
| 118 | Manipulating carriers' spin polarization in the Heusler alloy Mn ₂ CoAl. <i>RSC Advances</i> , 2015 , 5, 73814-73817 | 3.7 | 9 |
| 117 | Cooperative Gold Nanoparticle Stabilization by Acetylenic Phosphaalkenes. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 10634-8 | 16.4 | 13 |
| 116 | Theoretical assessment of feasibility to sequence DNA through interlayer electronic tunneling transport at aligned nanopores in bilayer graphene. <i>Scientific Reports</i> , 2015 , 5, 17560 | 4.9 | 35 |
| 115 | Towards a new class of heavy ion doped magnetic semiconductors for room temperature applications. <i>Scientific Reports</i> , 2015 , 5, 17053 | 4.9 | 14 |
| 114 | Nano-fabrication of molecular electronic junctions by targeted modification of metal-molecule bonds. <i>Scientific Reports</i> , 2015 , 5, 14431 | 4.9 | 18 |
| 113 | Stability of a new cubic monoxide of Thorium under pressure. <i>Scientific Reports</i> , 2015 , 5, 13740 | 4.9 | 6 |
| 112 | Effect of uniaxial strain on the site occupancy of hydrogen in vanadium from density-functional calculations. <i>Scientific Reports</i> , 2015 , 5, 10301 | 4.9 | 14 |
| 111 | Sensing Characteristics of a Graphene-like Boron Carbide Monolayer towards Selected Toxic Gases. <i>ChemPhysChem</i> , 2015 , 16, 3511-7 | 3.2 | 19 |
| 110 | Hydrogen Storage Materials for Mobile and Stationary Applications: Current State of the Art. <i>ChemSusChem</i> , 2015 , 8, 2789-825 | 8.3 | 236 |
| 109 | Improvement in hydrogen desorption from β - and γ -MgH ₂ upon transition-metal doping. <i>ChemPhysChem</i> , 2015 , 16, 2557-61 | 3.2 | 15 |
| 108 | Improvement in Hydrogen Desorption from β - and γ -MgH ₂ upon Transition-Metal Doping. <i>ChemPhysChem</i> , 2015 , 16, 2481-2481 | 3.2 | |
| 107 | Pressure-induced zigzag phosphorus chain and superconductivity in boron monophosphide. <i>Scientific Reports</i> , 2015 , 5, 8761 | 4.9 | 16 |
| 106 | Substitution induced band structure shape tuning in hybrid perovskites (CH ₃ NH ₃ Pb _{1-x} Sn _x I ₃) for efficient solar cell applications. <i>RSC Advances</i> , 2015 , 5, 107497-107502 | 3.7 | 37 |

| | | | |
|-----|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|-----|
| 105 | Polyfulvenes: Polymers with Bands That Enable Extensive Electronic Structure Tuning. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 25726-25737 | 3.8 | 12 |
| 104 | Pressure control of magnetic clusters in strongly inhomogeneous ferromagnetic chalcopyrites. <i>Scientific Reports</i> , 2015 , 5, 7720 | 4.9 | 10 |
| 103 | Disorder-induced room temperature ferromagnetism in glassy chromites. <i>Scientific Reports</i> , 2014 , 4, 4686 | 4.9 | 8 |
| 102 | A possible mechanism for the emergence of an additional band gap due to a TiO ₂ bond in the TiO ₂ /graphene hybrid system for enhanced photodegradation of methylene blue under visible light. <i>RSC Advances</i> , 2014 , 4, 59890-59901 | 3.7 | 113 |
| 101 | High-Pressure Phase Transition of ZnO Nanorods Using Density Functional Theory. <i>Integrated Ferroelectrics</i> , 2014 , 156, 122-128 | 0.8 | 1 |
| 100 | Strain Engineering for Phosphorene: The Potential Application as a Photocatalyst. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 26560-26568 | 3.8 | 314 |
| 99 | Design of High-Efficiency Visible-Light Photocatalysts for Water Splitting: MoS ₂ /AlN(GaN) Heterostructures. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 17594-17599 | 3.8 | 269 |
| 98 | Optical and electronic properties of nanosized BiTaO ₄ and BiNbO ₄ photocatalysts: Experiment and theory. <i>Physica Status Solidi (B): Basic Research</i> , 2014 , 251, 1034-1039 | 1.3 | 10 |
| 97 | Cerium; crystal structure and position in the periodic table. <i>Scientific Reports</i> , 2014 , 4, 6398 | 4.9 | 24 |
| 96 | Crafting ferromagnetism in Mn-doped MgO surfaces with p-type defects. <i>Science and Technology of Advanced Materials</i> , 2014 , 15, 035008 | 7.1 | 6 |
| 95 | Structural phase transition and metallization in compressed SrC ₂ . <i>Science Bulletin</i> , 2014 , 59, 5269-5271 | | 6 |
| 94 | Communication: Origin of the difference between carbon nanotube armchair and zigzag ends. <i>Journal of Chemical Physics</i> , 2014 , 140, 091102 | 3.9 | 10 |
| 93 | Electronic density-of-states of amorphous vanadium pentoxide films: Electrochemical data and density functional theory calculations. <i>Journal of Applied Physics</i> , 2014 , 115, 183701 | 2.5 | 14 |
| 92 | Revealing an unusual transparent phase of superhard iron tetraboride under high pressure. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014 , 111, 17050-3 | 11.5 | 20 |
| 91 | Layered Perovskite Sr ₂ Ta ₂ O ₇ for Visible Light Photocatalysis: A First Principles Study. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 5043-5050 | 3.8 | 41 |
| 90 | Atomistic study of promising catalyst and electrode material for memory capacitors: Platinum oxides. <i>Computational Materials Science</i> , 2013 , 79, 804-810 | 3.2 | 4 |
| 89 | Anion-Doped NaTaO ₃ for Visible Light Photocatalysis. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 22518-22524 | 3.5 | 63 |
| 88 | New type of possible high-pressure polymorphism in NiAs minerals in planetary cores. <i>Physics and Chemistry of Minerals</i> , 2013 , 40, 183-193 | 1.6 | 8 |

| | | | |
|----|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|-----|
| 87 | Tunable Assembly of sp ³ Cross-Linked 3D Graphene Monoliths: A First-Principles Prediction. <i>Advanced Functional Materials</i> , 2013 , 23, 5846-5853 | 15.6 | 49 |
| 86 | Transport coefficients in diamond from ab-initio calculations. <i>Applied Physics Letters</i> , 2013 , 102, 092106 | 3.4 | 5 |
| 85 | Single-layer MoS ₂ as an efficient photocatalyst. <i>Catalysis Science and Technology</i> , 2013 , 3, 2214 | 5.5 | 236 |
| 84 | Stabilizing a hexagonal Ru ₂ C via Lifshitz transition under pressure. <i>Applied Physics Letters</i> , 2013 , 103, 251901 | 3.4 | 11 |
| 83 | Improvement in the hydrogen desorption from MgH ₂ upon transition metals doping: A hybrid density functional calculations. <i>AIP Advances</i> , 2013 , 3, 102117 | 1.5 | 9 |
| 82 | Hybrid density functional study of electronic and optical properties of phase change memory material: Ge ₂ Sb ₂ Te ₅ . <i>Journal of Applied Physics</i> , 2013 , 113, 033510 | 2.5 | 13 |
| 81 | Pure and Li-doped NiTiH: Potential anode materials for Li-ion rechargeable batteries. <i>Applied Physics Letters</i> , 2013 , 103, 033902 | 3.4 | 11 |
| 80 | Role of correlation and relativistic effects in MAX phases. <i>Journal of Materials Science</i> , 2012 , 47, 7615-7620 | 2.0 | 14 |
| 79 | Oxygen- and nitrogen-chemisorbed carbon nanostructures for Z-scheme photocatalysis applications. <i>Journal of Nanoparticle Research</i> , 2012 , 14, 1 | 2.3 | 5 |
| 78 | Hybrid Density Functional and Molecular Dynamics Study of Promising Hydrogen Storage Materials: Double Metal Amidoboranes and Metal Amidoborane Ammoniates. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 17351-17359 | 3.8 | 6 |
| 77 | Strain induced lithium functionalized graphene as a high capacity hydrogen storage material. <i>Applied Physics Letters</i> , 2012 , 101, 103907 | 3.4 | 49 |
| 76 | Phase stability and superconductivity of strontium under pressure. <i>Applied Physics Letters</i> , 2012 , 101, 052604 | 3.4 | 2 |
| 75 | On the stability of single-walled carbon nanotubes and their binding strengths. <i>Theoretical Chemistry Accounts</i> , 2012 , 131, 1 | 1.9 | 7 |
| 74 | Study of electronic and optical properties of BiTaO ₄ for photocatalysis. <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , 2012 , 9, 1593-1596 | | 10 |
| 73 | Double-functionalized nanopore-embedded gold electrodes for rapid DNA sequencing. <i>Applied Physics Letters</i> , 2012 , 100, 023701 | 3.4 | 32 |
| 72 | HYDROGEN STORAGE ENHANCEMENT VIA TRANSITION METAL DECORATION ON METAL ORGANIC FRAMEWORKS: A FIRST-PRINCIPLES STUDY. <i>Nano</i> , 2012 , 07, 1250044 | 1.1 | 3 |
| 71 | Relativity and the lead-acid battery. <i>Physical Review Letters</i> , 2011 , 106, 018301 | 7.4 | 80 |
| 70 | Optical gap and native point defects in kaolinite studied by the GGA-PBE, HSE functional, and GW approaches. <i>Physical Review B</i> , 2011 , 84, | 3.3 | 25 |

| | | | |
|----|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|-----|
| 69 | Effective masses and electronic structure of diamond including electron correlation effects in first principles calculations using the GW-approximation. <i>AIP Advances</i> , 2011 , 1, 032139 | 1.5 | 28 |
| 68 | Enhanced DNA Sequencing Performance Through Edge-Hydrogenation of Graphene Electrodes. <i>Advanced Functional Materials</i> , 2011 , 21, 2674-2679 | 15.6 | 60 |
| 67 | Nanoelectrodes: Enhanced DNA Sequencing Performance Through Edge-Hydrogenation of Graphene Electrodes (Adv. Funct. Mater. 14/2011). <i>Advanced Functional Materials</i> , 2011 , 21, 2602-2602 | 15.6 | 3 |
| 66 | Theoretical investigation of xenon-hydrogen solids under pressure using ab initio DFT and GW calculations. <i>Physical Review B</i> , 2011 , 84, | 3.3 | 11 |
| 65 | Pressure-induced topological insulating behavior in the ternary chalcogenide Ge ₂ Sb ₂ Te ₅ . <i>Physical Review B</i> , 2011 , 84, | 3.3 | 35 |
| 64 | Origin of p-type conductivity in layered nGeTe _m Sb ₂ Te ₃ chalcogenide semiconductors. <i>Physical Review B</i> , 2011 , 83, | 3.3 | 33 |
| 63 | Origin of ferromagnetism in molybdenum dioxide from ab initio calculations. <i>Physical Review B</i> , 2010 , 81, | 3.3 | 14 |
| 62 | High-pressure phase transformations in carbonates. <i>Physical Review B</i> , 2010 , 82, | 3.3 | 23 |
| 61 | Differential conductance as a promising approach for rapid DNA sequencing with nanopore-embedded electrodes. <i>Applied Physics Letters</i> , 2010 , 97, 043701 | 3.4 | 13 |
| 60 | Hydrogen as promoter and inhibitor of superionicity: A case study on Li-N-H systems. <i>Physical Review B</i> , 2010 , 82, | 3.3 | 11 |
| 59 | Cumulene molecular wire conductance from first principles. <i>Physical Review B</i> , 2010 , 81, | 3.3 | 41 |
| 58 | Room temperature ferromagnetism in pristine MgO thin films. <i>Applied Physics Letters</i> , 2010 , 96, 232505 | 3.4 | 98 |
| 57 | One-dimensional polymeric carbon structure based on five-membered rings in alkaline earth metal dicarbides BeC ₂ and MgC ₂ . <i>Physical Review B</i> , 2010 , 82, | 3.3 | 26 |
| 56 | Understanding from First-Principles Why LiNH ₂ BH ₃ /NH ₃ BH ₃ Shows Improved Dehydrogenation over LiNH ₂ BH ₃ and NH ₃ BH ₃ . <i>Journal of Physical Chemistry C</i> , 2010 , 114, 19089-19095 | 3.8 | 26 |
| 55 | Epitaxial graphene monolayer and bilayers on Ru(0001): Ab initio calculations. <i>Physical Review B</i> , 2010 , 82, | 3.3 | 17 |
| 54 | Electronic Structure and High-Pressure Behavior of Solids 2010 , 269-290 | | |
| 53 | Li ⁺ ion conductivity and diffusion mechanism in Li ₃ N and Li ₃ N. <i>Energy and Environmental Science</i> , 2010 , 3, 1524 | 35.4 | 112 |
| 52 | Energetics and magnetic properties of V-doped MgO bulk and (001) surface: A GGA, GGA+U, and hybrid density functional study. <i>Physical Review B</i> , 2010 , 82, | 3.3 | 12 |

| | | | |
|----|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----|-----|
| 51 | Ab initio study on pressure-induced change of effective Coulomb interaction in superconducting yttrium. <i>Applied Physics Letters</i> , 2010 , 96, 022510 | 3.4 | 4 |
| 50 | Investigation on Ge ₅ Sb x Te ₅ phase-change materials by first-principles method. <i>Applied Physics A: Materials Science and Processing</i> , 2010 , 99, 961-964 | 2.6 | 4 |
| 49 | Superionicity in the hydrogen storage material Li ₂ NH: Molecular dynamics simulations. <i>Physical Review B</i> , 2009 , 79, | 3.3 | 20 |
| 48 | Energetics of Al doping and intrinsic defects in monoclinic and cubic zirconia: First-principles calculations. <i>Physical Review B</i> , 2009 , 80, | 3.3 | 25 |
| 47 | Non-transition-metal doped diluted magnetic semiconductors. <i>Applied Physics Letters</i> , 2009 , 94, 102504 | 3.4 | 60 |
| 46 | Thermodynamic analysis of hydrogen sorption reactions in LiMgNH systems. <i>Applied Physics Letters</i> , 2008 , 92, 021907 | 3.4 | 22 |
| 45 | Stable nitride complex and molecular nitrogen in N doped amorphous Ge ₂ Sb ₂ Te ₅ . <i>Applied Physics Letters</i> , 2008 , 93, 241908 | 3.4 | 32 |
| 44 | Fast crystallization of chalcogenide glass for rewritable memories. <i>Applied Physics Letters</i> , 2008 , 93, 061913 | 3.4 | 34 |
| 43 | Anisotropy in the electronic structure of V ₂ GeC investigated by soft x-ray emission spectroscopy and first-principles theory. <i>Physical Review B</i> , 2008 , 78, | 3.3 | 25 |
| 42 | Structurally induced insulator-metal transition in solid oxygen: A quasiparticle investigation. <i>Physical Review B</i> , 2008 , 77, | 3.3 | 17 |
| 41 | On the structural and energetic properties of the hydrogen absorber Li ₂ Mg(NH) ₂ . <i>Applied Physics Letters</i> , 2007 , 91, 091924 | 3.4 | 14 |
| 40 | Calculating carbon nanotube-catalyst adhesion strengths. <i>Physical Review B</i> , 2007 , 75, | 3.3 | 39 |
| 39 | Physisorption of nucleobases on graphene: Density-functional calculations. <i>Physical Review B</i> , 2007 , 76, | 3.3 | 274 |
| 38 | High-pressure structural transitions in Cm and Am _{0.5} Cm _{0.5} binary alloy. <i>High Pressure Research</i> , 2006 , 26, 377-381 | 1.6 | |
| 37 | Ab initio study of the Cr ₂ AlC(0001) surface. <i>Applied Physics Letters</i> , 2006 , 88, 161913 | 3.4 | 22 |
| 36 | Coupling in nanolaminated ternary carbides studied by theoretical means: The influence of electronic potential approximations. <i>Physical Review B</i> , 2006 , 73, | 3.3 | 45 |
| 35 | Resonant inelastic soft x-ray scattering at double core excitations in solid LiCl. <i>Physical Review B</i> , 2006 , 73, | 3.3 | 5 |
| 34 | ELECTRONIC STATES IN INTERCALATION MATERIALS STUDIED BY ELECTROCHEMICAL TECHNIQUES. <i>Modern Physics Letters B</i> , 2006 , 20, 863-875 | 1.6 | 8 |

| | | | |
|----|----------------------------------------------------------------------------------------------------------------------------------------------------------|-----|-----|
| 33 | Magnetoresistance and Hall-effect measurements of Ni thin films. <i>Journal of Applied Physics</i> , 2005 , 97, 083902 | 2.5 | 2 |
| 32 | Theoretical investigation of the bonding and elastic properties of nanolayered ternary nitrides. <i>Physical Review B</i> , 2005 , 71, | 3.3 | 105 |
| 31 | Stability of the MgCO ₃ structures under lower mantle conditions. <i>American Mineralogist</i> , 2005 , 90, 1008-1011 | 3.3 | 33 |
| 30 | High Pressure structural transitions in Cm metal. <i>Materials Research Society Symposia Proceedings</i> , 2005 , 893, 1 | | |
| 29 | Theoretical study of protactinium at high pressure. <i>Materials Research Society Symposia Proceedings</i> , 2005 , 893, 1 | | |
| 28 | Electronic, elastic, and optical properties of Y ₂ O ₂ S. <i>Journal of Applied Physics</i> , 2005 , 97, 103711 | 2.5 | 12 |
| 27 | Phase transitions in Am _{0.5} Cm _{0.5} binary alloy. <i>Materials Research Society Symposia Proceedings</i> , 2005 , 893, 1 | | |
| 26 | Resonant Inelastic Soft X-Ray Scattering at Hollow Lithium States in Solid LiCl. <i>Physical Review Letters</i> , 2004 , 93, | 7.4 | 5 |
| 25 | Titanium metal at high pressure: Synchrotron experiments and ab initio calculations. <i>Physical Review B</i> , 2004 , 69, | 3.3 | 46 |
| 24 | Calculated high pressure crystal structure transformations for phosphorus. <i>Physica Status Solidi (B): Basic Research</i> , 2003 , 235, 282-287 | 1.3 | 34 |
| 23 | High pressure structural phase transitions in IV-VI semiconductors. <i>Physica Status Solidi (B): Basic Research</i> , 2003 , 235, 341-347 | 1.3 | 39 |
| 22 | CRYSTALLOGRAPHIC STRUCTURES OF PbWO ₄ . <i>High Pressure Research</i> , 2003 , 23, 343-347 | 1.6 | 12 |
| 21 | H-H interaction and structural phase transition in Ti ₃ SnH _x . <i>Physical Review B</i> , 2002 , 66, | 3.3 | 4 |
| 20 | Cotunnite-Structured Titanium Dioxide and the Hardest known Oxide. <i>High Pressure Research</i> , 2002 , 22, 429-433 | 1.6 | 7 |
| 19 | High Pressure Theoretical Studies of Actinide Dioxides. <i>High Pressure Research</i> , 2002 , 22, 471-474 | 1.6 | 24 |
| 18 | Reduction of shock-wave data with mean-field potential approach. <i>Journal of Applied Physics</i> , 2002 , 92, 6616-6620 | 2.5 | 42 |
| 17 | Ab initio calculations of the mechanical properties of Ti ₃ SiC ₂ . <i>Applied Physics Letters</i> , 2001 , 79, 1450-1452 | 3.4 | 71 |
| 16 | Theoretical prediction of a phase transition in gold. <i>Physical Review B</i> , 2001 , 63, | 3.3 | 31 |

| | | | |
|----|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|-----|
| 15 | Experimental and theoretical identification of a new high-pressure TiO ₂ polymorph. <i>Physical Review Letters</i> , 2001 , 87, 275501 | 7.4 | 156 |
| 14 | First Principles Simulations of Phase Stability in Stoichiometric and Doped LiMnO ₂ . <i>Materials Research Society Symposia Proceedings</i> , 2001 , 677, 4161 | | |
| 13 | High pressure studies of sodium and silver halides. <i>High Pressure Research</i> , 2000 , 18, 131-138 | 1.6 | |
| 12 | Ab initio calculation of elastic constants of SiO ₂ stishovite and quartz. <i>Journal of Chemical Physics</i> , 1999 , 111, 2071-2074 | 3.9 | 40 |
| 11 | Eine Erklärung für die eigentliche Elementstruktur von Indium. <i>Angewandte Chemie</i> , 1999 , 111, 2155-2159 | 9.6 | 4 |
| 10 | The Origin of the Distorted Close-Packed Elemental Structure of Indium. <i>Angewandte Chemie - International Edition</i> , 1999 , 38, 2017-2020 | 16.4 | 19 |
| 9 | Melting and liquid structure of aluminum oxide using a molecular-dynamics simulation. <i>Physical Review E</i> , 1998 , 57, 1673-1676 | 2.4 | 45 |
| 8 | Anomalous fcc crystal structure of thorium metal. <i>Physical Review Letters</i> , 1995 , 75, 280-283 | 7.4 | 31 |
| 7 | Theoretical confirmation of the high pressure simple cubic phase in calcium. <i>Physical Review Letters</i> , 1995 , 75, 3473-3476 | 7.4 | 68 |
| 6 | Electronic structure of platinum at ultrahigh pressure. <i>High Pressure Research</i> , 1994 , 12, 161-170 | 1.6 | 6 |
| 5 | Asymmetry-Induced Redistribution in Sn(IV)/Ti(IV) Hetero-Bimetallic Alkoxide Precursors and Its Impact on Thin-Film Deposition by Metal-Organic Chemical Vapor Deposition. <i>Crystal Growth and Design</i> , | 3.5 | 0 |
| 4 | Molecular nanoinformatics approach assessing the biocompatibility of biogenic silver nanoparticles with channelized intrinsic steatosis and apoptosis. <i>Green Chemistry</i> , | 10 | 4 |
| 3 | Dimensionality effects in high-performance thermoelectric materials: Computational and experimental progress in energy harvesting applications. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , e1547 | 7.9 | 3 |
| 2 | Electric Field-Modulated Charge Transfer in Geometrically Tailored MoX ₂ /WX ₂ (X = S, Se) Heterostructures. <i>Journal of Physical Chemistry C</i> , | 3.8 | 4 |
| 1 | Nanolayered MAX Phases from Ab Initio Calculations | 199-204 | 3 |