# Abir De Sarkar

List of Publications by Year
in descending order

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|---|---|---|---|
| 88 papers | 3,113 citations | 172207 29 h-index | 174990 52 g-index |
| 88 all docs | 88 docs citations | 88 times ranked | 3815 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | A comprehensive study on carrier mobility and artificial photosynthetic properties in group VI B transition metal dichalcogenide monolayers. Journal of Materials Chemistry A, 2018, 6, 8693-8704. | 5.2 | 204 |
| 2 | TiO<sub>2</sub>-Based Gas Sensor: A Possible Application to SO<sub>2</sub>. ACS Applied Materials & Interfaces, 2013, 5, 8516-8522. | 4.0 | 186 |
| 3 | Direct Observation of Molecular Orbitals of Pentacene Physisorbed on Au(111) by Scanning Tunneling Microscope. Physical Review Letters, 2009, 102, 176102. | 2.9 | 135 |
| 4 | Emergence of high piezoelectricity along with robust electron mobility in Janus structures in semiconducting Group IVB dichalcogenide monolayers. Journal of Materials Chemistry A, 2018, 6, 24885-24898. | 5.2 | 127 |
| 5 | A porous, crystalline truxene-based covalent organic framework and its application in humidity sensing. Journal of Materials Chemistry A, 2017, 5, 21820-21827. | 5.2 | 115 |
| 6 | Nanoscale Interfaces of Janus Monolayers of Transition Metal Dichalcogenides for 2D Photovoltaic and Piezoelectric Applications. Journal of Physical Chemistry C, 2020, 124, 10385-10397. | 1.5 | 94 |
| 7 | Group-IV(A) Janus dichalcogenide monolayers and their interfaces straddle gigantic shear and in-plane piezoelectricity. Nanoscale, 2021, 13, 5460-5478. | 2.8 | 89 |
| 8 | Ultrahigh Out-of-Plane Piezoelectricity Meets Giant Rashba Effect in 2D Janus Monolayers and Bilayers of Group IV Transition-Metal Trichalcogenides. Journal of Physical Chemistry C, 2020, 124, 21250-21260. | 1.5 | 87 |
| 9 | Solar Energy Harvesting in Type II van der Waals Heterostructures of Semiconducting Group III Monochalcogenide Monolayers. Journal of Physical Chemistry C, 2019, 123, 12666-12675. | 1.5 | 86 |
| 10 | Interfacing Boron Monophosphide with Molybdenum Disulfide for an Ultrahigh Performance in Thermoelectrics, Two-Dimensional Excitonic Solar Cells, and Nanopiezotronics. ACS Applied Materials & Interfaces, 2020, 12, 3114-3126. | 4.0 | 84 |
| 11 | Comparison of the full-potential and frozen-core approximation approaches to density-functional calculations of surfaces. Physical Review B, 2006, 73, . | 1.1 | 80 |
| 12 | Interfacial hybridization of Janus MoSSe and BX (X = P, As) monolayers for ultrathin excitonic solar cells, nanopiezotronics and low-power memory devices. Nanoscale, 2020, 12, 22645-22657. | 2.8 | 73 |
| 13 | Manipulating Molecular Quantum States with Classical Metal Atom Inputs: Demonstration of a Single Molecule NOR Logic Gate. ACS Nano, 2011, 5, 1436-1440. | 7.3 | 72 |
| 14 | Proton-Triggered Fluorescence Switching in Self-Exfoliated Ionic Covalent Organic Nanosheets for Applications in Selective Detection of Anions. ACS Applied Materials & Interfaces, 2020, 12, 13248-13255. | 4.0 | 69 |
| 15 | Nano-structured hybrid molybdenum carbides/nitrides generated in situ for HER applications. Journal of Materials Chemistry A, 2017, 5, 7764-7768. | 5.2 | 64 |
| 16 | Single-phase Ni<sub>5</sub>P<sub>4</sub>â€“copper foam superhydrophilic and aerophobic coreâ€“shell nanostructures for efficient hydrogen evolution reaction. Journal of Materials Chemistry A, 2019, 7, 23989-23999. | 5.2 | 58 |
| 17 | Strain induced lithium functionalized graphane as a high capacity hydrogen storage material. Applied Physics Letters, 2012, 101, . | 1.5 | 55 |
| 18 | Strain Induced Band Dispersion Engineering in Si Nanosheets. Journal of Physical Chemistry C, 2011, 115, 23682-23687. | 1.5 | 54 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Superhigh out-of-plane piezoelectricity, low thermal conductivity and photocatalytic abilities in ultrathin 2D van der Waals heterostructures of boron monophosphide and gallium nitride. Nanoscale, 2019, 11, 21880-21890. | 2.8 | 54 |
| 20 | ZrS3/MS2 and ZrS3/MXY (M Mo, W; X, Y S, Se, Te; Xâ€¯â‰¤â€¯Y) type-II van der Waals hetero-bilayers: Prospective candidates in 2D excitonic solar cells. Applied Surface Science, 2020, 499, 143894. | 3.1 | 51 |
| 21 | Giant tunability in electrical contacts and doping via inconsiderable normal electric field strength or gating for a high-performance in ultrathin field effect transistors based on 2D BX/graphene (XÂ=ÂP,) Tj ETQq1 1 0.784314 rgBT /Ov | | |
| 22 | Strain-Induced Optimization of Nanoelectromechanical Energy Harvesting and Nanopiezotronic Response in a MoS<sub>2</sub> Monolayer Nanosheet. Journal of Physical Chemistry C, 2017, 121, 9181-9190. | 1.5 | 50 |
| 23 | Shear strain induced indirect to direct transition in band gap in AlN monolayer nanosheet. Computational Materials Science, 2014, 86, 206-210. | 1.4 | 44 |
| 24 | Tweaking the Physics of Interfaces between Monolayers of Buckled Cadmium Sulfide for a Superhigh Piezoelectricity, Excitonic Solar Cell Efficiency, and Thermoelectricity. ACS Applied Materials & Interfaces, 2020, 12, 18123-18137. | 4.0 | 44 |
| 25 | Functionalization of hydrogenated graphene by polylithiated species for efficient hydrogen storage. International Journal of Hydrogen Energy, 2014, 39, 2560-2566. | 3.8 | 40 |
| 26 | Strain and pH facilitated artificial photosynthesis in monolayer MoS<sub>2</sub> nanosheets. Journal of Materials Chemistry A, 2017, 5, 22265-22276. | 5.2 | 40 |
| 27 | Compressive strain induced enhancement in thermoelectric-power-factor in monolayer MoS<sub>2</sub>nanosheet. Journal of Physics Condensed Matter, 2017, 29, 225501. | 0.7 | 38 |
| 28 | Hot Hole Cooling and Transfer Dynamics from Lead Halide Perovskite Nanocrystals Using Porphyrin Molecules. Journal of Physical Chemistry C, 2021, 125, 5859-5869. | 1.5 | 37 |
| 29 | Coupled spin and valley polarization in monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Hf</mml:mi><mml:msub><mml:mi mathvariant="normal">N</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> and valley-contrasting physics at the <mml:math | 1.1 | 35 |
| 30 | Effective modulation of ohmic contact and carrier concentration in a graphene- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Mg</mml:mi><mml:mi>X</mml:mi></mml:mrow></mml: ( <mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 307 Td (xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:m | 1.1 | 30 |
| 31 | Re Hydrogen storage in polylithiated BC3 monolayer sheet. Solid State Communications, 2013, 170, 39-43. | 0.9 | 29 |
| 32 | Enhancement of energy storage capacity of Mg functionalized silicene and silicane under external strain. Applied Physics Letters, 2014, 105, . | 1.5 | 29 |
| 33 | Electronic and transport behavior of doped armchair silicene nanoribbons exhibiting negative differential resistance and its FET performance. RSC Advances, 2017, 7, 12783-12792. | 1.7 | 29 |
| 34 | Two-dimensional ultrathin van der Waals heterostructures of indium selenide and boron monophosphide for superfast nanoelectronics, excitonic solar cells, and digital data storage devices. Nanotechnology, 2020, 31, 495208. | 1.3 | 29 |
| 35 | Nano-hives for plant stimuli controlled targeted iron fertilizer application. Chemical Engineering Journal, 2019, 375, 121995. | 6.6 | 28 |
| 36 | Electrochemically customized assembly of a hybrid xerogel materialviacombined covalent and non-covalent conjugation chemistry: an approach for boosting the cycling performance of pseudocapacitors. Journal of Materials Chemistry A, 2020, 8, 6740-6756. | 5.2 | 28 |

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| 37 | Valley drift and valley current modulation in strained monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Mo</mml:mi><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2019, 100, . | 1.1 | 27 |
| 38 | CO oxidation and NO reduction over supported Pt-Rh and Pd-Rh nanocatalysts: a comparative study. Journal of Molecular Catalysis A, 2005, 229, 25-29. | 4.8 | 26 |
| 39 | Spin-Current Modulation in Hexagonal Buckled ZnTe and CdTe Monolayers for Self-Powered Flexible-Piezo-Spintronic Devices. ACS Applied Materials & Interfaces, 2021, 13, 40872-40879. | 4.0 | 26 |
| 40 | A comparative and a systematic study on the effects of B, N doping and C-atom vacancies on the band gap in narrow zig-zag graphene nanoribbons via quantum transport calculations. Materials Research Bulletin, 2017, 87, 167-176. | 2.7 | 25 |
| 41 | Electronic structure modification of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>KTaO</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:m surface by<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:mi>Ar</mml:mi></mml:mrow><mml:mo>+</mml:m Physical Review B, 2017, 96, | 1.1 | 25 |
| 42 | Experimental and Theoretical Study into Interface Structure and Band Alignment of the Cu<sub>2</sub>Zn<sub>1â€“x</sub>Cd<sub>x</sub>SnS<sub>4</sub> Heterointerface for Photovoltaic Applications. ACS Applied Energy Materials, 2020, 3, 5153-5162. | 2.5 | 25 |
| 43 | 2D HfN2/graphene interface based Schottky device: Unmatched controllability in electrical contacts and carrier concentration via electrostatic gating and out-of-plane strain. Applied Surface Science, 2021, 540, 148389. | 3.1 | 25 |
| 44 | Excited state properties of Si quantum dots. Physica Status Solidi (B): Basic Research, 2012, 249, 401-412. | 0.7 | 24 |
| 45 | Strain-induced tunability of optical and photocatalytic properties of ZnO mono-layer nanosheet. Computational Materials Science, 2014, 91, 38-42. | 1.4 | 22 |
| 46 | Superhigh flexibility and out-of-plane piezoelectricity together with strong anharmonic phonon scattering induced extremely low lattice thermal conductivity in hexagonal buckled CdX (X =) Tj ETQq0 0 0 rgBT /Overlock 10 T | 0.7 | 22 |
| 47 | Ultra-low lattice thermal conductivity and giant phononâ€“electric field coupling in hafnium dichalcogenide monolayers. Journal of Physics Condensed Matter, 2020, 32, 315301. | 0.7 | 22 |
| 48 | Ultra-low thermal conductivity and super-slow hot-carrier thermalization induced by a huge phononic gap in multifunctional nanoscale boron pnictides. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 124, 114222. | 1.3 | 21 |
| 49 | Electronic Structure Modulation of 2D Colloidal CdSe Nanoplatelets by Au25 Clusters for High-Performance Photodetectors. Journal of Physical Chemistry C, 2020, 124, 19793-19801. | 1.5 | 20 |
| 50 | Valley spin polarization in two-dimensional <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>h</mml:mi><mml:mtext>â^’</mml:mtext><mml:mi>M</m mathvariant="normal">N</mml:mi></mml:mrow><mml:mo>Â</mml:mo><mml:mrow><mml:mo>(</mml:mo><mml:mi>M</mml:mi><m monolayers: Merger of valleytronics with spintronics. Physical Review B, 2022, 105, . | 1.1 | 20 |
| 51 | Controlled formation of nanostructures on MoS2 layers by focused laser irradiation. Applied Physics Letters, 2017, 110, 083101. | 1.5 | 19 |
| 52 | Conflux of tunable Rashba effect and piezoelectricity in flexible magnesium monochalcogenide monolayers for next-generation spintronic devices. Nanoscale, 2021, 13, 8210-8223. | 2.8 | 19 |
| 53 | A systematic investigation of acetylene activation and hydracyanation of the activated acetylene on Au<sub>n</sub> (n = 3â€“10) clusters via density functional theory. Physical Chemistry Chemical Physics, 2016, 18, 13830-13843. | 1.3 | 18 |
| 54 | Exceptional mechano-electronic properties in the HfN<sub>2</sub> monolayer: a promising candidate in low-power flexible electronics, memory devices and photocatalysis. Physical Chemistry Chemical Physics, 2020, 22, 21275-21287. | 1.3 | 18 |

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|---|---|---|---|
| 55 | Interfacing 2D M2X (MÂ=ÂNa, K, Cs; XÂ=ÂO, S, Se, Te) monolayers for 2D excitonic and tandem solar cells. Applied Surface Science, 2021, 563, 150304. | 3.1 | 18 |
| 56 | Surface-nitrogenationâ€“induced thermal conductivity attenuation in silicon nanowires. Europhysics Letters, 2011, 96, 56007. | 0.7 | 15 |
| 57 | Lithium storage in amorphous TiNi hydride: Electrode for rechargeable lithium-ion batteries. Materials Chemistry and Physics, 2013, 141, 348-354. | 2.0 | 15 |
| 58 | The role of exfoliating solvents for control synthesis of few-layer graphene-like nanosheets in energy storage applications: Theoretical and experimental investigation. Applied Surface Science, 2020, 509, 145375. | 3.1 | 15 |
| 59 | Atomistic manipulation of interfacial properties in HfN2/MoTe2 van der Waals heterostructure via strain and electric field for next generation multifunctional nanodevice and energy conversion. Applied Surface Science, 2021, 568, 150928. | 3.1 | 15 |
| 60 | Insights into CrS2 monolayer and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si6.svg"><mml:mi>n</mml:mi></mml:math>-CrS2/<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si7.svg"><mml:mi>p</mml:mi></mml:math>-HfN2 interface for low-power digital and analog nanoelectronics. Applied Surface Science, 2022, 579, 152211. | 3.1 | 14 |
| 61 | Strain and doping effects on the energetics of hydrogen desorption from the MgH <sub>2</sub> (001) surface. Europhysics Letters, 2013, 101, 27006. | 0.7 | 13 |
| 62 | Influence of Boron Substitution on Conductance of Pyridine- and Pentane-Based Molecular Single Electron Transistors: First-Principles Analysis. Journal of Electronic Materials, 2016, 45, 2233-2241. | 1.0 | 12 |
| 63 | Polylithiated (OLi2) functionalized graphane as a potential hydrogen storage material. Applied Physics Letters, 2012, 101, 243902. | 1.5 | 11 |
| 64 | First-principles study on the origin of ferromagnetism in n-type Cu-doped ZnO. Solid State Communications, 2012, 152, 1057-1060. | 0.9 | 11 |
| 65 | Pure and Li-doped NiTiH: Potential anode materials for Li-ion rechargeable batteries. Applied Physics Letters, 2013, 103, 033902. | 1.5 | 11 |
| 66 | Tailoring the transmission lineshape spectrum of zigzag graphene nanoribbon based heterojunctions via controlling their width and edge protrusions. Nanoscale, 2015, 7, 20003-20008. | 2.8 | 11 |
| 67 | Dual response of graphene-based ultra-small molecular junctions to defect engineering. Nano Research, 2016, 9, 1480-1488. | 5.8 | 10 |
| 68 | Influence of sulphur on the shell composition of Ptâ€“Rh nanocatalysts: a theoretical model. Chemical Physics Letters, 2002, 353, 426-430. | 1.2 | 9 |
| 69 | Improvement in the desorption of H2 from the MgH2 (110) surface by means of doping and mechanical strain. Computational Materials Science, 2014, 86, 165-169. | 1.4 | 9 |
| 70 | Screening study of light-metal and transition-metal-doped NiTiH hydrides as Li-ion battery anode materials. Solid State Ionics, 2014, 258, 88-91. | 1.3 | 9 |
| 71 | Electronic and Vibrational Properties of Stable Isomers of (SiO)<sub>n</sub><sup>(0,Â±)</sup> (n = 2â€“7) Clusters. Journal of Physical Chemistry A, 2014, 118, 8893-8900. | 1.1 | 9 |
| 72 | Electronic Band Structure and Ultrafast Carrier Dynamics of Two Dimensional (2D) Semiconductor Nanoplatelets (NPLs) in the Presence of Electron Acceptor for Optoelectronic Applications. Journal of Physical Chemistry C, 2020, 124, 26434-26442. | 1.5 | 9 |

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|---|---|---|---|
| 73 | Size dependent catalytic effect of TiO2 clusters in water dissociation. Journal of Molecular Catalysis A, 2013, 366, 163-170. | 4.8 | 8 |
| 74 | Effect of metalâ€“support interaction on surface segregation in Pdâ€“Pt nanoparticles. Applied Surface Science, 2001, 182, 394-397. | 3.1 | 7 |
| 75 | Conformational dependence of tag induced intramolecular STM contrast in hexaphenylbenzene molecules. Surface Science, 2009, 603, L57-L61. | 0.8 | 7 |
| 76 | Strain-induced stabilization of Al functionalization in graphene oxide nanosheet for enhanced NH3 storage. Applied Physics Letters, 2013, 102, . | 1.5 | 7 |
| 77 | Intramolecular Torsion Based Molecular Switch Functionality Enhanced in Ï€-Conjugated Oligomolecules by a Ï€-Conjugated Pendant Group. Journal of Physical Chemistry C, 2011, 115, 13911-13918. | 1.5 | 6 |
| 78 | Inducing novel electronic properties in âŒ©112âŒª Ge nanowires by means of variations in their size, shape and strain: a first-principles computational study. Journal of Physics Condensed Matter, 2012, 24, 015301. | 0.7 | 6 |
| 79 | The effects of different possible modes of uniaxial strain on the tunability of electronic and band structures in $$ext {MoS}_2$$ MoS 2 monolayer nanosheet via first-principles density functional theory. Pramana - Journal of Physics, 2017, 89, 1. | 0.9 | 6 |
| 80 | Microkinetic model studies of impurity effects on CO+O2, CO+NO and CO+NO+O2 reactions over supported Ptâ€“Rh nanocatalysts. Chemical Physics Letters, 2004, 384, 339-343. | 1.2 | 5 |
| 81 | Electronic charge transport through ZnO nanoribbons. Journal of Physics and Chemistry of Solids, 2014, 75, 1223-1228. | 1.9 | 5 |
| 82 | Hexagonal Boron Nitride Sheet Decorated by Polylithiated Species for Efficient and Reversible Hydrogen Storage. Science of Advanced Materials, 2013, 5, 1960-1966. | 0.1 | 5 |
| 83 | Effects of temperature and adsorbates on the composition profile of Ptâ€“Rh nanocatalysts: a comparative study. Physica B: Condensed Matter, 2002, 315, 82-87. | 1.3 | 4 |
| 84 | Impact of transverse and vertical gate electric field on vibrational and electronic properties of MoS2. Journal of Applied Physics, 2020, 127, . | 1.1 | 3 |
| 85 | The electronic transparency of a single CO molecule at contact. Chemical Physics Letters, 2010, 484, 237-241. | 1.2 | 2 |
| 86 | Concurrence of negative in-plane piezoelectricity and photocatalytic properties in 2D ScAgP<sub>2</sub>S<sub>6</sub> monolayers. Journal of Physics Condensed Matter, 2021, 33, 375301. | 0.7 | 2 |
| 87 | IMPURITY AND SUPPORT EFFECTS ON SURFACE COMPOSITION AND CO+NO REACTIONS OVER Ptâ€“Rh/CeO2 NANOPARTICLES: A COMPARATIVE STUDY. International Journal of Modern Physics B, 2003, 17, 4831-4839. | 1.0 | 1 |
| 88 | CHARACTERISTIC VIBRATIONAL MODES OF H2O ADSORBED MOLECULARLY AND DISSOCIATIVELY ON TITANIUM OXIDE CLUSTERS. Journal of Theoretical and Computational Chemistry, 2012, 11, 1289-1295. | 1.8 | 1 |