## Biswajit Saha

List of Publications by Year in descending order

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**ΒΙςνηνιτ ζ**άμα

#	Article	IF	CITATIONS
1	Carbonization in Polyacrylonitrile (PAN) Based Carbon Fibers Studied by ReaxFF Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2012, 116, 4684-4692.	2.6	140
2	Extraordinary Improvement of the Graphitic Structure of Continuous Carbon Nanofibers Templated with Double Wall Carbon Nanotubes. ACS Nano, 2013, 7, 126-142.	14.6	84
3	Highly Sensitive Bendable and Foldable Paper Sensors Based on Reduced Graphene Oxide. ACS Applied Materials & Interfaces, 2017, 9, 4658-4666.	8.0	73
4	A review on the importance of surface coating of micro/nano-mold in micro/nano-molding processes. Journal of Micromechanics and Microengineering, 2016, 26, 013002.	2.6	63
5	Singly and doubly excited states of butadiene, acrolein, and glyoxal: Geometries and electronic spectra. Journal of Chemical Physics, 2006, 125, 014316.	3.0	54
6	Multi-step mechanism of carbonization in templated polyacrylonitrile derived fibers: ReaxFF model uncovers origins of graphite alignment. Carbon, 2015, 94, 694-704.	10.3	54
7	Hot Giant Fullerenes Eject <i>and</i> Capture C <sub>2</sub> Molecules: QM/MD Simulations with Constant Density. Journal of Physical Chemistry C, 2011, 115, 22707-22716.	3.1	47
8	Quantum Chemical Molecular Dynamics Simulations of Dynamic Fullerene Self-Assembly in Benzene Combustion. ACS Nano, 2009, 3, 2241-2257.	14.6	46
9	Multiscale Simulation as a Framework for the Enhanced Design of Nanodiamond-Polyethylenimine-Based Gene Delivery. Journal of Physical Chemistry Letters, 2012, 3, 3791-3797.	4.6	42
10	Investigation of the Electronic Spectra and Excited-State Geometries of Poly(para-phenylene vinylene) (PPV) and Poly(para-phenylene) (PP) by the Symmetry-Adapted Cluster Configuration Interaction (SAC-CI) Method. Journal of Physical Chemistry A, 2007, 111, 5473-5481.	2.5	30
11	Formation mechanism of polycyclic aromatic hydrocarbons in benzene combustion: Quantum chemical molecular dynamics simulations. Journal of Chemical Physics, 2010, 132, 224303.	3.0	25
12	Chemical Dynamics Simulations of Energy Transfer for Propylbenzene Cation and He Collisions. Journal of Physical Chemistry A, 2017, 121, 7494-7502.	2.5	14
13	Interaction and thermal stability of carboxymethyl cellulose on α-Fe2O3(001) surface: ReaxFF molecular dynamics simulations study. Journal of Molecular Graphics and Modelling, 2021, 102, 107787.	2.4	14
14	Coexistence of Normal and Auxetic Behavior in a Thermally and Chemically Stable sp <sup>3</sup> Nanothread: Poly[5]asterane. Chemistry - A European Journal, 2017, 23, 12917-12923.	3.3	12
15	Reactive Molecular Dynamics Simulations of Self-Assembly of Polytwistane and Its Application for Nanofibers. Journal of Physical Chemistry C, 2018, 122, 19204-19211.	3.1	11
16	Antineoplastic properties of zafirlukast against hepatocellular carcinoma via activation of mitochondrial mediated apoptosis. Regulatory Toxicology and Pharmacology, 2019, 109, 104489.	2.7	11
17	A study on frictional behavior of PMMA against FDTS coated silicon as a function of load, velocity and temperature. Tribology International, 2016, 102, 44-51.	5.9	9
18	Ultra‣ensitive and Highly Stretchable Strain Sensors for Monitoring of Human Physiology. Macromolecular Materials and Engineering, 2022, 307, 2100666.	3.6	9

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19	Environmental application of amine functionalised magnetite nanoparticles grafted graphene oxide chelants. Environmental Science and Pollution Research, 2022, 29, 86485-86498.	5.3	9
20	Hot-embossing performance of silicon micromold coated with self-assembled n-octadecyltrichlorosilane. Sensors and Actuators B: Chemical, 2011, 160, 207-214.	7.8	8
21	Insights on the initial stages of carbonization of sub-bituminous coal. Journal of Molecular Graphics and Modelling, 2021, 106, 107868.	2.4	7
22	PDMS Sylgard 527-Based Freely Suspended Ultrathin Membranes Exhibiting Mechanistic Characteristics of Vascular Basement Membranes. ACS Applied Materials & Interfaces, 2018, 10, 40388-40400.	8.0	6
23	Magnetic Nanoparticle Encapsulation for the Manipulation of Bacterial Movement and Spontaneous Detection by Reduced Graphene Oxide. Advanced Biology, 2018, 2, 1800095.	3.0	6
24	Highâ€resolution costâ€effective compact portable inverted light microscope. Journal of Microscopy, 2019, 273, 199-209.	1.8	6
25	Reduced graphene oxide-based stretchable strain sensor for monitoring of physical activities and minute movement. Materials Today: Proceedings, 2022, 62, 5975-5981.	1.8	6
26	Theoretical Studies of the O( <sup>3</sup> P) + C <sub>2</sub> Reaction at Hyperthermal Energies. Journal of Physical Chemistry C, 2012, 116, 26577-26585.	3.1	5
27	Interaction of Grafted Dextrin with a Hematite Surface: Effect of Functional Groups and Molecular Weight. ChemistrySelect, 2021, 6, 8165-8170.	1.5	5
28	Synthesis of magnetite-graphene nanocomposite for wastewater treatment. Materials Today: Proceedings, 2022, 62, 6042-6048.	1.8	5
29	Macromolecular selective flocculant derived from functionalized starch towards beneficiation of low-quality iron ore: Atomistic simulations and experimental studies. Materials Today Communications, 2022, 32, 103810.	1.9	5
30	Titanium–aluminum–polytetrafluoroethylene coated stainless steel micromold via co-sputtering deposition: Replication performance and limitation in hot-embossing. Sensors and Actuators B: Chemical, 2012, 163, 290-298.	7.8	4
31	Adsorption mechanism and performance analysis of alkaloids as green corrosion inhibitors on mild steel. Theoretical Chemistry Accounts, 2022, 141, .	1.4	1