

Recent Research Publications

Title of Paper	Authors	UGC referred or Not	Indexing	Publisher	Name of Journal	Impact Factor	H-Index	Affiliation
Enhancement of Schiff base biological efficacy by metal coordination and introduction of metallic compounds as anticovid candidates: a simple overview.	Mir, J. M., Majid, S. A., & Shalla, A. H.	yes	<u>SCI/SCIE Indexed</u>	De gruyter	<i>Reviews in Inorganic Chemistry</i>	5.79	29	IUST
PEDOT and PEDOT: PSS conducting polymeric hydrogels: A report on their emerging applications	Bhat, M. A., Rather, R. A., & Shalla, A. H.	Yes	<u>SCI/SCIE Indexed</u>	Elsevier	<i>Synthetic Metals</i>	4.4	150	IUST
Synthesis and characterization of Mo (0) and W (0) complexes of bis (azol-1-yl) methane based bis-phosphines.	Bhat, S. A., Sonawane, S. C., Mague, J. T., & Balakrishna, M. S.	Yes	<u>SCI/SCIE Indexed</u>	Taylor & Francis	<i>Journal of Coordination Chemistry</i>	2.3	59	IUST
Synthesis of novel 2,5-bis(substituted thio)-1,3,4-thiadiazoles by acid catalyzed intermolecular cyclization reactions of substituted dithiocarbazates as a possible 2019-nCoV main protease inhibitor.	Bhat, M.A. Jan, M. Manzoor, U. Shalla, A. H Butcher, R. J. Jasinski, J. P.	Yes	<u>SCI/SCIE Indexed</u>	Elsevier	<i>Journal of Molecular Structure</i>	3.8	117	IUST
A Nonclinical spectroscopic approach for diagnosing covid-19: a concise perspective.	Mir, J. M., Khan, M. W., Shalla, A. H., & Maurya, R. C.	Yes	<u>SCI/SCIE Indexed</u>	Springer	<i>Journal of Applied Spectroscopy</i>	0.7	29	IUST
Nitric oxide as a therapeutic option for COVID-19 treatment: a concise perspective.	Mir, J. M., & Maurya, R. C.	Yes	<u>SCI/SCIE Indexed</u>	RSC	<i>New Journal of Chemistry</i>	4	131	IUST
Solid state electron density aspects of mordenite with experimentally evaluated nitrate and phosphate sorption.	Mir, J. M., Mir, M. A., Majid, S. A., & Malik, B. A	Yes	<u>SCI/SCIE Indexed</u>	Elsevier	<i>Materials Science and Engineering: B</i>	6.4	135	IUST
Thermodynamics of cosolvent effect of surface-active ionic liquids on the micellization of conventional surfactant	Farooq, U., Malik, N. A., & Shalla, A. H.	Yes	<u>SCI/SCIE Indexed</u>	Springer	<i>Colloid and Polymer Science</i>	2.4	95	IUST
Interactions of tricyclic antidepressant drug chlomipramine hydrochloride with imidazolium based surface active ionic liquid in aqueous solution.	Malik, N. A., Farooq, U., Rather, M. A., & Shalla, A. H.	Yes	<u>SCI/SCIE Indexed</u>	Elsevier	<i>Journal of Molecular Liquids</i>	6.27	150	IUST

Molecular scaffolds from mother nature as possible lead compounds in drug design and discovery against coronaviruses: A landscape analysis of published literature and molecular docking studies.	Khursheed, A., Jain, V., Rasool, A., Rather, M. A., Malik, N. A., & Shalla, A. H.	Yes	<u>SCI/SCIE Indexed</u>	Elsevier	<i>Microbial Pathogenesis</i>	3.8	98	IUST
Multicomponent interpenetrating metal-based Alginate-Carrageenan biopolymer hydrogel beads substantiated by graphene oxide for efficient removal of methylene blue from waste water.	Rather, R. A., Bhat, M. A., & Shalla, A. H.	Yes	<u>SCI/SCIE Indexed</u>	Elsevier	<i>Chemical Engineering Research and Design</i>	4.29	125	IUST
Viscoelastic and smart swelling disposition of Carboxymethylcellulose based hydrogels substantiated by Gemini surfactant and in-vitro encapsulation and controlled release of Quercetin.	Bhat, M. A., Rather, R. A., Yaseen, Z., & Shalla, A. H.	Yes	<u>SCI/SCIE Indexed</u>	Elsevier	<i>International Journal of Biological Macromolecules</i>	8.87	191	IUST
Smart polyacrylamide– cholic acid hybrid composite hydrogel: development, characterization, and encapsulation study of methylene blue dye.	Bhat, M. A., Rangreez, T. A., Yaseen, Z., Rather, R. A., & Shalla, A. H.	Yes	<u>SCI/SCIE Indexed</u>	Elsevier	<i>Materials Today Communications</i>	4.06	55	IUST
Texture and rheological features of strain and pH sensitive chitosan-imine graphene-oxide composite hydrogel with fast self-healing nature.	Bhat, M. A., Rather, R. A., & Shalla, A. H.	Yes	<u>SCI/SCIE Indexed</u>	Elsevier	<i>International Journal of Biological Macromolecules</i>	8.87	191	IUST
Tantalum based single, double, and triple atom catalysts supported on gC ₂ N monolayer for effective nitrogen reduction reaction: a comparative DFT investigation.	Rasool, A., Anis, I., Dixit, M., Maibam, A., Hassan, A., Krishnamurty, S., & Dar, M. A.	Yes	<u>SCI/SCIE Indexed</u>	RSC	<i>Catalysis Science & Technology</i>	6	145	IUST
Electrocatalytic nitrogen reduction directed through the p-band center of boron on B SAC@ Mo ₂ C	Maibam, A., Krishnamurty, S., & Dar, M. A.	Yes	<u>SCI/SCIE Indexed</u>	RSC	<i>Materials Advances</i>	5	42	IUST
First-Principles Investigation of the Electrocatalytic Reduction of CO ₂ on Zirconium-Based Single-, Double-, and Triple-Atom Catalysts Anchored on a Graphitic Carbon Nitride Monolayer.	Hassan, A., Anis, I., Shafi, S., Assad, A., Rasool, A., Khanam, R., Bhat, G. A.; Krishnamurty, S.; Dar, M. A.	Yes	<u>SCI/SCIE Indexed</u>	ACS	<i>ACS Applied Nano Materials</i>	6	64	IUST

Probing the Site-Specific Reactivity and Catalytic Activity of Ag _n (n= 15–20) Silver Clusters	Anis, I., Dar, M. S., Bhat, G. A., Rather, G. M., & Dar, M. A.	Yes	<u>SCI/SCIE Indexed</u>	ACS	<i>ACS omega</i>	4	77	IUST
Role of magnetization on catalytic pathways of non-oxidative methane activation on neutral iron carbide clusters.	Kumar, M., Dar, M. A., Katiyar, A., Agrawal, R., Shenai, P. M., & Srinivasan, V.	Yes	<u>SCI/SCIE Indexed</u>	RSC	<i>Physical Chemistry Chemical Physics</i>	3.3	290	IUST
Exploring the structure and electronic properties of germanium doped boron clusters using density functional theory based global optimization method	Anis, I., Dar, M. S., Rather, G. M., & Dar, M. A.	Yes	<u>SCI/SCIE Indexed</u>	RSC	<i>New Journal of Chemistry</i>	4	131	IUST
Glucosamine and maltol anchored Zinc (II) complex of COVID-19 health supplement relevance: DFT collaborated spectroscopic formulation with profound biological implications.	Mir, J. M., Malik, B. A., & Khan, M. W.	Yes	<u>SCI/SCIE Indexed</u>	Elsevier	<i>Journal of the Indian Chemical Society</i>	1.65	35	IUST
Schiff base complexes, cancer cell lines, and anticancer evaluation: a review	Majid, S. A., Mir, J. M., Jan, G., & Shalla, A. H.	Yes	<u>SCI/SCIE Indexed</u>	Taylor & Francis	<i>Journal of Coordination Chemistry</i>	2.3	59	IUST
A novel tetrahedral silver complex of (z)-o-methyl s-hydrogen tosylcarbonimidothioate: DFT supported crystallographic and spectroscopic study.	Mir, J. M., Khan, M. W., & Diwan, K.	Yes	<u>SCI/SCIE Indexed</u>	Elsevier	<i>Journal of the Indian Chemical Society</i>	1.65	35	IUST
NO, CO and H ₂ S based pharmaceuticals in the mission of vision (eye health): a comprehensive review.	Mir, J. M., Maurya, R. C., & Khan, M. W.	Yes	<u>SCI/SCIE Indexed</u>	De gruyter	<i>Reviews in Inorganic Chemistry</i>	5.79	29	IUST
Nitric oxide boosters as defensive agents against COVID-19 infection: an opinion.	Mir, J. M., & Maurya, R. C.	Yes	<u>SCI/SCIE Indexed</u>	Taylor & Francis	<i>Journal of Biomolecular Structure and Dynamics</i>	6.25	87	IUST
Drug Solubilization by Surfactants: Experimental Methods and Theoretical Perspectives	Malik, N.A.	Yes	<u>SCI/SCIE Indexed</u>	Bentham Science	<i>Mini Reviews in Medicinal Chemistry</i>	4.02	107	IUST
Effect of caffeine on the micellization and related thermodynamic parameters of sodium dodecyl sulphate, hexadecyltrimethylammonium bromide and triton x-100: a physicochemical study.	Malik, N. A., & Farooq, U.	Yes	<u>SCI/SCIE Indexed</u>	Taylor & Francis	<i>Physics and Chemistry of Liquids</i>	1.53	38	IUST

Plant based natural products as potential ecofriendly and safer biopesticides: A comprehensive overview of their advantages over conventional pesticides, limitations and regulatory aspects.	Khursheed, A., Rather, M. A., Jain, V., Rasool, S., Nazir, R., Malik, N. A., & Majid, S. A.	Yes	<u>SCI/SCIE Indexed</u>	Elsevier	<i>Microbial Pathogenesis</i>	3.8	98	IUST
Influence of HSA on micellization of NLSS and BC: An experimental-theoretical approach of its binding characteristics.	Fatma, I., Sharma, V., Malik, N. A., Assad, H., Cantero-López, P., Sánchez, J., ... & Kumar, A.	Yes	<u>SCI/SCIE Indexed</u>	Elsevier	<i>Journal of Molecular Liquids</i>	6.27	150	IUST
Development of sodium alginate-guar-gum-tannic acid based nanocomposite hydrogel beads for removal of malachite green dye.	Rather, R. A., Bhat, M. A., & Shalla, A. H.	Yes	<u>SCI/SCIE Indexed</u>	Elsevier	<i>Materials Today Communications</i>	4.06	55	IUST
N ₂ Activation and Reduction on Graphdiyne Supported Single, Double, and Triple boron Atom Catalysts: A First Principles Investigation	Anis, I., Amin, S., Rather, G. M., & Dar, M. A.	Yes	<u>SCI/SCIE Indexed</u>	Wiley	<i>ChemistrySelect</i>	2.23	51	IUST
Implications of the Pore Size of Graphitic Carbon Nitride Monolayers on the Selectivity of Dual-Boron Atom Catalysts for the Reduction of N ₂ to Urea and Ammonia: A Computational Investigation	Dar, M. A.	Yes	<u>SCI/SCIE Indexed</u>	ACS	<i>Inorganic Chemistry</i>	4.6	246	IUST
Assessing the Suitability of α -SiS Nanosheet as an Anode Material for Multivalent Metal-Ion Batteries.	Shaikh, G. A., Cornil, D., Dar, M. A., Gupta, S. K., Ahuja, R., & Gajjar, P. N.	Yes	<u>SCI/SCIE Indexed</u>	ACS	<i>Energy & Fuels</i>	5.52	221	IUST
Optimizing the NRR activity of single and double boron atom catalysts using a suitable support: a first principles investigation.	Rasool, A., Anis, I., Bhat, S. A., & Dar, M. A.	Yes	<u>SCI/SCIE Indexed</u>	RSC	<i>Physical Chemistry Chemical Physics</i>	3.43	290	IUST
Understanding the activity of single atom catalysts for CO ₂ reduction to C ₂ products: A high throughput computational screening.	Hassan, A., & Dar, M. A.	Yes	<u>SCI/SCIE Indexed</u>	RSC	<i>New Journal of Chemistry</i>	4	131	IUST
Boosting CO ₂ Activation and Reduction by Engineering the Electronic Structure of Graphitic Carbon Nitride through Transition Metal-Free Single-Atom Functionalization.	Fozia, S., Hassan, A., Reshi, S. A., Singh, P., Bhat,	Yes	<u>SCI/SCIE Indexed</u>	ACS	<i>Journal of Physical Chemistry C</i>	3.7	257	IUST

	G. A., Dixit, M., & Dar, M. A.							
Nickel single atom catalyst supported on the gallium nitride monolayer: first principles investigations on the decisive role of support in the electrocatalytic reduction of CO ₂ .	Khanam, R., Hassan, A., Nazir, Z., & Dar, M. A.	Yes	<u>SCI/SCIE Indexed</u>	ACS	<i>Sustainable Energy & Fuels</i>	5.6	75	IUST
Synthesis, structural analysis, DFT and molecular docking studies of N-(6-(((E)-4-methoxybenzylidene)amino)hexyl)-1-(4-methoxyphenyl) methanimine and its hydrate as a possible 2019-nCoV protease inhibitor.	Bhat, M. A. Wani, O. A. Bhat, S. A. Butcher, R. J	Yes	<u>SCI/SCIE Indexed</u>	Elsevier	<i>Journal of Molecular Structure</i>	3.8	117	IUST
Design, Synthesis, Molecular Docking, and In Vitro Antibacterial Evaluation of Benzotriazole-Based β -Amino Alcohols and Their Corresponding 1, 3-Oxazolines	Singh, N., Abrol, V., Parihar, S., Kumar, S., Khanum, G., Mir, J. M., & Al-Farraj, S.	Yes	<u>SCI/SCIE Indexed</u>	ACS	<i>ACS omega</i>	4	77	IUST
A pair of carbazate derivatives as novel Schiff base ligands: DFT and POM theory supported spectroscopic and biological evaluation.	Majid, S. A., Mir, J. M., Bhat, M. A., Shalla, A. H., Pandey, A., Hadda, T. B., & Abdellattif, M. H.	Yes	<u>SCI/SCIE Indexed</u>	Taylor & Francis	<i>Journal of Biomolecular Structure and Dynamics</i>	6.25	87	IUST
Electronic structure, phonon stability, mechanical and high-temperature thermoelectric properties of Li-based quaternary Heusler alloys.	Singh, J., Kaur, K., Islam, I., Mir, J. M., Goyal, M., Kaur, T., & Khandy, S. A.	Yes	<u>SCI/SCIE Indexed</u>	Elsevier	<i>Current Applied Physics</i>	2.4	91	IUST
Synthesis and DFT supported spectroscopic characterization of a pyrazolone Schiff base complex of RuII-NO core.	Mir, J. M., & Maurya, R. C.	Yes	<u>SCI/SCIE Indexed</u>	Taylor & Francis	<i>Inorganic and Nano-metal Chemistry</i>	2	51	IUST
Influence of Antidepressant Drug on the Conductivity of Cationic Surfactant.	Malik, N. A., Farooq, U., Malik, A., & Rather, M. A.	Yes	<u>SCI/SCIE Indexed</u>	Springer	<i>Colloid Journal</i>	1.18	38	IUST

Computational identification of most potent atom pair catalysts for electrocatalytic nitrogen reduction reaction over hydrogen evolution reaction	Verma, T. S., Dar, A. H., Dar, M. A., Selvaraj, K., & Krishnamurty, S.	Yes	<u>SCI/SCIE Indexed</u>	Elsevier	<i>International Journal of Hydrogen Energy</i>	3.8	117	IUST
Structure-directing interactions in the crystals of tertiary butyl carbazate based imines: A combined experimental and theoretical investigation.	Bhat, M. A. Anis I. Almarhoon, Z. M. Bhat, S. A. Jan, M. Dar, M. A. Butcher, R. J.	Yes	<u>SCI/SCIE Indexed</u>	Elsevier	<i>Journal of Molecular Structure</i>	3.8	117	IUST