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السيرة الذاتية

الاسم	**محمد رمضان جانجوعة**
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التخصص	الكيمياء الفيزيائية
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المواقع الالكترونية

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https://scholar.google.com.pk/citations?hl=en&user=Rw_bxq8AAAAJ&view_op=list_works&s%20ortby=pubdate.

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أولاً / المؤهلات العلمية:

2003: MBA Marketing, Preston Institute of Management Science & Technology (PIMSAT), Pakistan
2001: B.Sc. Chemistry, Zoology and Botany, University of the Punjab, Pakistan
2005: M.Sc. Physical Chemistry, Chemistry Department, University of Sargodha, Pakistan)
:2010Ph.D. Physical Chemistry, Chemistry Department, Northeast Normal University, China .
Dissertation Title: "A quantum mechanical investigation of electronic properties in Lindqvist-type polyoxometalate derivatives: Organic-inorganic hybrid functional materials" Advisor: Prof. Zhongmin Su (zmsu@nenu.edu.cn)

PROFESSIONAL EXPERIENCE **الخبرات العلمية**

Dec 2022 – till today: Professor, Chemistry Department, Government College University Faisalabad (GCUF) Pakistan (BPS-21) .
May 2022 – Aug. 2022: Professor, Chemistry Department, King Fahd University of Petroleum & Minerals, Dhahran, Kingdom of Saudi Arabia (Foreign Contract-21).
Apr. 2018 – May 2022: Associate Professor, Chemistry Department, King Fahd University of Petroleum & Minerals, Dhahran, Kingdom of Saudi Arabia (Foreign Contract-20) .
Jan. 2016 – Apr. 2018: Assistant Professor, Chemistry Department, King Fahd University of Petroleum & Minerals, Dhahran, Kingdom of Saudi Arabia (Foreign Contract-19)
Nov. 2010 – Jan. 2016: Assistant Professor, Chemistry Department, University of Sargodha, Sargodha, Pakistan* (BPS-19)
Aug. 2010 – Nov. 2010: Assistant Professor, Chemistry Department, G. C. University

Faisalabad, Faisalabad, Pakistan (IPFPs-19)

Apr. 2011 – Apr. 2012: Post-Doc, University of Coimbra, Portugal

*Experience letter verified by Saudi Embassy and Ministry of Foreign Affair and letters of promotion at the rank of Associate Professor/Professor provided at the end of this CV.

Publications المنشورات

Journal #	PUBLICATIONS at the rank of FULL PROFESSOR at KFUPM	Impact Factor/Quartile* (Year Published)
J150	M.R.S.A. Janjua*, Z. Shafiq, S. Shahzadi, U. Rehman, S. Shoukat, R. Azeem, S.H. Ali, L.K.M.O. Goni, Recent Developments and Future Challenges for Perovskite Solar Cells: Physical Insights to Improve PCE, Braz.J.Phys, (2024) 54(4), 134. https://doi.org/10.1007/s13538-024-01526-7	1.36/Q4 X
J149	I. Hussain, M.R.S.A. Janjua*, A.U Haq, S.U. Hassan, F.M.K. Albaqami, M.A. Alsuwat, B.M. Alrashdi, S. Alzwain, S.A.R. Naqvi, Evaluation of Anti-Infection and Anti-Diabetic Activities in Methanolic and n-Hexane Plant Extracts of Indigenously Cultivated Chenopodium album, Agronomy, (2024) 14(7),1340. https://doi.org/10.3390/agronomy14071340	3.7/Q1 W
J148	S.A.R. Naqvi, A.J. Hassan, M.R.S.A. Janjua*, N. Abbas, A.F. Zahoor, S.U. Hassan, A. Hussain, Radiolabeling and preclinical animal model evaluation of DTPA coupled 99mTc-labelled flutamide complex ([99mTc] DTPA-FLUT) as a potential radiotracer for cancer imaging, Acta Radiologica, (2024) 02841851241249161. https://doi.org/10.1177/02841851241249161	1.701/Q3 W
J147	A. Mahmood, S. Naeem, A. Javed, Z. Shafiq, M.A. El-Sheikh, H.O. Elansary, M.R.S.A. Janjua*, Chemical similarity-based design of materials for organic solar cells: Visualizing the generated chemical space of polymers, Mater. Today Commun, (2024) 38, 108403. https://doi.org/10.1016/j.mtcomm.2024.108403	4.06/Q2 W
J146	T. Mubashir, M.H. Tahir, Z. Shafiq, A.Z. Dewidar, H.O. El-ansary, M.R.S.A. Janjua*, An efficient framework to design near-IR monomers for polymer solar cells with the help of machine learning, virtual screening and chemical space visualization, J. Photochem. Photobiol. A, (2024) 447, 115285. https://doi.org/10.1016/j.jphotochem.2023.115285	5.141/Q1 W
J145	M.A.Z.G. Sial, M. Mateen, R. Naz, M. Abbas, N. Abbas, S.H. Talib, M.R.S.A. Janjua*, Mohammad Qamar, Alloying platinum single atoms with nickel iron nanoalloys for high performance hydrogen evolution reaction, Int. J. Hydrog. Energy, (2024) 51, 540-549. https://doi.org/10.1016/j.ijhydene.2023.06.291	7.67/Q1 W
J144	W.A. Gill, N. Alhokbany, M.R. S.A. Janjua*, Adsorption of molecular hydrogen on $Be_3Al_2(SiO_3)$ 6-beryl: theoretical insights for catalysis, hydrogen storage, gas separation, sensing, and environmental applications, RSC Adv. (2024) 14(6), 3782-3789. 10.1039/D3RA07480C	3.9/Q2 W
J143	W.A. Gill, M.T. Aziz, H.W. Darwish, M.R.S.A. Janjua*, Exploring HCl–HCl interactions: QZVPP calculations, improved Lennard-Jones potential, and second virial coefficient analysis for thermodynamics and industrial applications, RSC Adv. (2024) 14(3), 1890-1901. 10.1039/D3RA04387H	3.9/Q2 W
J142	M.U. Khan, S. Nadeem, A. Fatima, J. Yaqoob, F. Abbas, H.W. Darwish, M.R.S.A. Janjua*, Theoretical study of static and frequency-dependent nonlinear optical	

	properties of 1-phenyl-2, 5-di (thiophen-2-yl)-1H-pyrrole based D-π-A chromophores through π-linkers modifications: A gateway towards giant nonlinear optical compounds, Mater. Sci. Eng. B, (2024) 299, 116993. https://doi.org/10.1016/j.mseb.2023.116993	4.682/Q2 W
J141	M.U. Khan, F. Shafiq, M.R.S.A. Janjua*, M. Khalid, J. Yaqoob, M. Arshad, S.M. Alshehri, R.A. Khan, Predicting benzodithiophene based donor materials with enhanced 19.09% PCE, open-circuit voltage and optoelectronic attributes for solar cell applications: Photochemical insights from DFT, J. Photochem. Photobiol. A, (2024) 446, 115115. https://doi.org/10.1016/j.jphotochem.2023.115115	5.141/Q1 W
J140	M.A.Z.G. Sial, M. Mateen, R. Naz, M. Abbas, N. Abbas, S.H. Talib, M.R.S.A. Janjua*, M. Qamar, Alloying platinum single atoms with nickel iron nanoalloys for high performance hydrogen evolution reaction, Int. J. Hydrog. Energy, (2024) 31, 540-549. https://doi.org/10.1016/j.ijhydene.2023.06.291	7.67/Q1 W
J139	M.A. Afzal, M.U. Khan, M.U. Alvi, J. Yaqoob, N. Alhokbany, S. Ahmed, M.R.S.A. Janjua*, Exploring novel naphthalene-fused octacyclic core-based non-fullerene acceptor materials with augmented optoelectronic attributes for stable and efficient solar cells, J. Mol. Struct. (2024) 1295, 136646. https://doi.org/10.1016/j.molstruc.2023.136646	3.841/Q2 X
J138	B. Basha, M. Sulaman, S. Elshahat, H.M. Jafri, Z.A. Alrowaili, M.S. Al-Buriahi, M.R.S.A. Janjua*, Multidimensional modelling and designing of efficient small molecule acceptors for organic solar cells, Mater. Sci. Eng. B, (2023) 296, 116618. https://doi.org/10.1016/j.mseb.2023.116618	4.682/Q2 W
J137	S. Jamil, S.R. Khan, S. Bibi, N. Jahan, N. Mushtaq, F. Rafaqat, R.A. Khan, W.A. Gill, M.R.S.A. Janjua*, Recent advances in synthesis and characterization of iron–nickel bimetallic nanoparticles and their applications as photo-catalyst and fuel additive, RSC Adv. (2023) 13(42), 29632-29644. 10.1039/D3RA04293F	3.9/Q2 W
J136	S. Jamil, S.R. Khan, S. Ali, S. Bibi, R.A. Khan, W.A. Gill, M.R.S.A. Janjua, Synthesis of calcium-bismuth layered double hydroxide (LADH) Nanoparticles: Applications as Photo-catalyst and Fuel Additive, Inorg. Chem. Commun. (2023) 157, 1111331. https://doi.org/10.1016/j.inoche.2023.111331	3.800/Q2 X
J135	A. Asif, M.U. Khan, J. Yaqoob, G. Mustafa, S. Ahmed, N. Alhokbany, Z. Shafiq, M.R.S.A. Janjua, Tuning nonlinear optical properties of tetracyclopentatetraphenylnene by superhalogens doping: Quantum chemical perspective of novel NLO materials for modern optoelectronic applications, Mater. Sci. Eng. B, (2023) 297, 116763. https://doi.org/10.1016/j.mseb.2023.116763	4.682/Q2 W
J134	F. Bano, J. Yaqoob, R. Hussain, M. Bourass, N. Alhokbany, Z. Shafiq, M.R.S.A. Janjua*, M.U. Khan, Doping superalkalis on chlorine substituted coronene: Interactive design computation of new NLO materials for optoelectronics, J. Photochem. Photobiol. A, (2023) 442, 114810. https://doi.org/10.1016/j.jphotochem.2023.114810	5.141/Q1 W
J133	Z. Shafiq, S.A.R. Naqvi, M.R.S.A. Janjua, S. Jamil, First Theoretical Engineering of Robust C-C Single bond-based Acceptor Materials for Efficient Organic Photovoltaics, J. Photochem. Photobiol. A, (2023) 442,114782. https://doi.org/10.1016/j.jphotochem.2023.114782	5.141/Q1 W
J132	W.A. Gill, M.R.S.A. Janjua*, Ab Initio Calculations of the Interaction Potential of the N_2O–N_2O Dimer: Strength of the Intermolecular Interactions and Physical Insights, J. Phys. Chem. A, (2023) 127(30), 6175-6185. https://doi.org/10.1021/acs.jpca.3c02634	2.900/Q2 Y

J131	M.U. Khan, S. Nadeem, A. Fatima, J. Yaqoob, M. Khalid, F. Abbas, N. Alhokbany, M.R.S.A. Janjua, DFT molecular simulations for static, dynamic and solvent-dependent nonlinear optical properties of triphenylamine-carbazole-based organic dyes with DDA framework, J. Mol. Liq. (2023) 391, 123258. https://doi.org/10.1016/j.molliq.2023.123258	6.27/Q1 W
J130	W.A. Gill, M.R.S.A. Janjua*, Exploring the Adsorption Mechanism of N_2O on Graphene: A DFT Study on Circum-Coronene for Catalysis, Sensing, and Energy Storage Applications, J. Phys. Chem. A, (2023) 127(26), 5591–560. https://doi.org/10.1021/acs.jpca.3c03133	2.900/Q2 Y
J129	T. Hassan, I. Sajid, M.R.S.A. Janjua, Z. Shafiq, M.Y. Mehboob, N. Sultan, Non-fullerene based photovoltaic materials for solar cell applications: DFT-based Analysis and Interpretation, Comput. Theor. Chem, (2023) 1224, 114128 https://doi.org/10.1016/j.comptc.2023.114128	6.578/Q1 Y
J128	M.U. Khan, M.R.S.A. Janjua, J. Yaqoob, R. Hussain, M. Khalid, A. Syed, A.M. Elgorban, N.S.S. Zaghloul, First theoretical framework of superalkali metals [M_3X (M= Li, Na, k; X= O, S, F, N)] doped all-boron B38 nanocluster: A promising class of nonlinear optical materials for optoelectronic applications, J. Photochem. Photobiol. A, (2023) 440,114667. https://doi.org/10.1016/j.jphotochem.2023.114667	5.141/Q1 W
J127	M.R.S.A. Janjua, Impact of symmetry breaking on the performance of non-fullerene acceptors (NFAs) for photo and thermally stable organic solar cells (OSCs): a DFTbased interrogation and investigation, J. Photochem. Photobiol. A, (2023) 444, 115003. https://doi.org/10.1016/j.jphotochem.2023.115003	5.141/Q1 W
J126	M.Y. Mehboob, R. Hussain, F. Younas, S. Jamil, M.M.A. Iqbal, K. Ayub, N. Sultana, M.R.S.A. Janjua*, Computation assisted design and prediction of alkali-metal-centered B12N12 nanoclusters for efficient H2 adsorption: New hydrogen storage materials, J. Clust. Sci. (2023) 34(4), 1237-1247. https://doi.org/10.1007/s10876-022-02294-7	3.447/Q2 X
J125	S. Jamil, S.R. Khan, S. Bibi, N. Jahan, N. Mushtaq, F. Rafaqat, R.A. Khan, W.A. Gill, M.R.S.A. Janjua*, Exploring the adsorption behavior of molecular hydrogen on CHA-zeolite by comparing the performance of various force field methods, RSC Adv. (2023), 13(42), 30937-30950. https://doi.org/10.1039/D3RA04262F	3.9/Q2 W
J124	T. Mubashir, M.H.Tahir, M.H.H. Mahmoud, Z. Shafiq, M. Ashraf, I.H. El. Azab, Z.M. El-Bahy, M.R.S.A. Janjua*, Designing of symmetric and asymmetric small molecule acceptors for organic solar cells: A farmwork based on Machine learning, virtual screening and structural analysis, J. Photochem. Photobiol. A, (2023) 444, 114977. https://doi.org/10.1016/j.jphotochem.2023.114977	5.141/Q1 W
J123	S. Jamil, A.R. Alvi, S. Bibi, N. Jahan, S.A.R. Naqvi, S.R. Khan, K.M. Zia, M.R.S.A. Janjua*, Synthesis, characterization, and applications of cobalt bismuth layered double hydroxide nanoparticles: Physical insights towards a potential material as fuel additive and photocatalyst, J. Phys. Org. Chem, (2023) 36(7), e4500. https://doi.org/10.1002/poc.4500	2.155/Q4 X
J122	N. Sultana, M. Sarfraz, S. Akram, U. Rashid, S.A.R. Naqvi, M.I. Tariq, K.M. Zia, M.R.S.A. Janjua*, Reactivity of 2, 2-disubstituted quinazolinone towards electrophilic substitution: First in silico design to verify experimental evidence of quinazolinonebased new organic compounds, J. Phys. Org. Chem, (2023) 36(5), e4488. https://doi.org/10.1002/poc.4488	2.155/Q4 X
J121	O.A.A. Ali, M.U. Khan, M.A. Asghar, S.F. Mahmoud, S.M. El-Bahy, R. Baby, M.R.S.A. Janjua*, A new cyano (−C ≡ N) free molecular design perspective for	

	constructing carbazole-thiophene based environmental friendly organic solar cells, Phys. B: Condens. Matter. (2023) 652, 414630. https://doi.org/10.1016/j.physb.2022.414630	2.988/Q2 X
J120	S. Jamil, G. Zahra and M.R.S.A. Janjua*, Morphologically controlled synthesis, characterization, and applications of molybdenum oxide (MoO_3) nanoparticles, J. Phys. Org. Chem., (2023), 36(4), e4477. https://doi.org/10.1002/poc.4477	2.155/Q4 X
J119	M.R.S.A. Janjua*, Photovoltaic properties and enhancement in near-infrared light absorption capabilities of acceptor materials for organic solar cell applications: A quantum chemical perspective via DFT, J. Phys. Chem. Solids, (2022) 110996. https://doi.org/10.1016/j.jpcs.2022.110996	4.383/Q2 W
J118	M.R.S.A. Janjua*, All-small-molecule organic solar cells with high fill factor and enhanced open-circuit voltage with 18.25 % PCE: Physical insights from quantum chemical calculations, Spectrochim. Acta A Mol. Biomol. Spectrosc. (2022) 121487. https://doi.org/10.1016/j.saa.2022.121487	4.831/Q1 W
J117	I. Shahbaz, S. Jamil, S. Bibi, S.R. Khan, and M.R.S.A. Janjua*, Recent Advances in Morphologically Controlled Synthesis of Graphene Oxide Based Nanocomposite as Catalyst and Fuel Additive, J. Phys. Org. Chem. (2022) 35/10, e4409 https://doi.org/10.1002/poc.4409	2.155/Q4 X
J116	A. Umar, J. Yaqoob, M.U. Khan, R. Hussain, A.A. Abdulraheem. S.A. Almalki, M.R.S.A. Janjua*, Doping of superalkali and superhalogen on graphene quantum dot surfaces to enhance nonlinear optical response: An efficient strategy for fabricating novel electro-optical materials, J. Phys. Chem. Solids (2022) 169, 110859 https://doi.org/10.1016/j.jpcs.2022.110859	4.383/Q2 W
J115	S.J.U.H. Shah, S. Jamil, S. Ali, S.R. Khan, M.R.S.A. Janjua, Synthesis of Rod Like Chromium/Manganese Layer Double Hydroxide and Applications, Russ. J. Phys. Chem. A.(2022) 96, 1215–1227 https://doi.org/10.1134/S0036024422060218	0.791/Q4 Y
J114	M Haroon, W. Fatima, M.R.S.A. Janjua*, Physicochemical insights into the rational designing of new acceptor molecules by donor bridge modifications for efficient solar cells: In silico chemistry, J. Phys. Org. Chem. (2022) 35/10, e4399 https://doi.org/10.1002/poc.4399	2.155/Q4 X
J113	S. Naz, G. Bibi, S. Jamil, S. UrRehman, S. Bibi, S. Ali, T. Khan, S.R. Khan, M.R.S.A. Janjua, Preparation of manganese-doped tin oxide nanoparticles for catalytic reduction of organic dyes, Chem. Phys. Lett. (2022) 802, 139768 https://doi.org/10.1016/j.cplett.2022.139768	2.719/Q3 X
J112	M.Y. Mehboob, R. Hussain, F. Younas, S. Jamil, M.M.A. Iqbal, K. Ayub, N. Sultana, M.R.S.A. Janjua*, Computation Assisted Design and Prediction of Alkali-Metal-Centered $B_{12}N_{12}$ Nanoclusters for Efficient H_2 Adsorption: New Hydrogen Storage Materials, J. Clust. Sc. (2022) https://doi.org/10.1007/s10876-022-02294-7	3.447/Q2 X
J111	M. Haroon, S. Jamil, M.B. Zeshan, N. Sultana, M.I. Tariq, M.R.S.A. Janjua*, Photovoltaic Properties of Hole Transport Materials for Organic Solar Cells (OSCs) Applications: Physiochemical Insight and In Silico Designing, Aust. J. Chem. (2022) 75/6, 399-411 https://doi.org/10.1071/CH22029	1.224/Q4 X
J110	M.B. Zeshan, N. Sultana, M. I. Tariq. S. Jamil and M.R.S.A. Janjua*, Physicochemical insights and in silico designing of new fullerene-free acceptor molecules for highly efficient and stable organic solar cells, J. Phys. Chem. Solids, (2022) 169, 110842 https://doi.org/10.1016/j.jpcs.2022.110842	4.383/Q2 W

	PUBLICATIONS at the rank of ASSOCIATE PROFESSOR at KFUPM	
J109	M.R.S.A. Janjua*, Quantum chemical design and prediction that complements understanding: How do the transition metals enhance the CO_2 sensing ability of inorganic $Mg_{12}O_{12}$ nanoclusters? J. Phys. Chem. Solids (2022) 167, 110789 https://doi.org/10.1016/j.jpcs.2022.110789	4.383/Q2 W
J108	G Bibi, SR Khan, S Ali, S Jamil, S Bibi, H Shehroz, M.R.S.A. Janjua, Role of capping agent in the synthesis of zinc–cobalt bimetallic nanoparticles and its application as catalyst and fuel additive, Appl. Nanosci, (2022) 12, 2169–2181 https://doi.org/10.1007/s13204-022-02468-9	3.869/Q3 NA
J107	M Haroon, M.R.S.A. Janjua*, Computationally Assisted Design and Prediction of Remarkably Boosted NLO Response of Organoimido-Substituted Hexamolybdates J. Phys. Org. Chem., (2022) 35/8, e4353 https://doi.org/10.1002/poc.4353	2.391/Q3 X
J106	A Irfan, M Hussien, MY Mehboob, A Ahmad, M.R.S.A. Janjua*, Learning from fullerenes and predicting for Y6. Machine learning and high-throughput screening of small molecule donors for organic solar cells, Energy Technol., (2022) 10/6, 101096 https://doi.org/10.1002/ente.202101096	3.631/Q3 W
J105	M.R.S.A Janjua, A Irfan, M Hussien, M Ali, M Saqib, M Sulaman, Machine-Learning Analysis of Small-Molecule Donors for Fullerene Based Organic Solar Cells, Energy Technol., (2022) 10/5, 2200019 https://doi.org/10.1002/ente.202200019	3.631/Q3 W
J104	Q. UlAin, S. Ali, S. Jamil, S. Bibi, S.R. Khan, S. UrRehman, G. Bibi, T. Khan, H. Shehroz, M. Hashaam, M.R.S.A. Janjua, Comparison of catalytic and fuel additive properties of bimetallic nanoparticles and its composite: FeMnO3 and PANI-FeMnO3, Mater. Sci. Semicond. Process, (2022) 144, 106630 https://doi.org/10.1016/j.mssp.2022.106630	3.927/Q2 W
J103	M.R.S.A. Janjua*, Quantum Design of Transition Metals Decorated on Boron Phosphide Inorganic Nanocluster for Favipiravir Adsorption: A Possible Treatment for Covid-19, New J. Chem. (2022) 46, 1720-1730 https://doi.org/10.1039/D1NJ04697G	3.591/Q2 W
J102	M. Y. Mehboob, R. Hussain, S. Jamil, M. Ahmed, M. U. Khan, M. Haroon, M.R.S.A. Janjua*, Physical-Organic Aspects along with Linear and Nonlinear Optical Properties of Benzene Sulfonamide Compounds: In Silico Analysis, J. Phys. Org. Chem. (2022) 35/4, e4313 https://doi.org/10.1002/poc.4313	2.391/Q3 X
J101	M. Y. Mehboob, R. Zaier, R. Hussain, M. A. Malik, M. A. Iqbal, Z. Irshad, I. Bilal, M.R.S.A. Janjua*, In Silico Modelling of Acceptor Materials by End-capped and π-linker modifications for High Performance Organic Solar Cells: Estimated PCE > 18% Comp. Theor. Chem. (2022) 1208, 113555 https://doi.org/10.1016/j.comptc.2021.113555	1.926/Q4 X
J100	M. Haroon, M.R.S.A. Janjua*, Exploring the effect of end-capped modifications of carbazole-based fullerene-free acceptor molecules for high-performance indoor organic solar cell applications, J. Comput. Electron. (2022) 21, 40–51 https://doi.org/10.1007/s10825-021-01838-w	1.807/Q3 X
J99	M. Haroon, A. A. Al-Saadi, M.R.S.A. Janjua*, Insights into end-capped modifications effect on the photovoltaic and optoelectronic properties of S-shaped fullerene-free acceptor molecules: A density functional theory computational study for organic solar cells, J. Phys. Org. Chem. (2022) 35/4, e4314 https://doi.org/10.1002/poc.4314	2.391/Q3 X
J98	M. Y. Mehboob, R. Hussain, M. Adnan, Saira, U. Farwa, Z. Irshad, M.R.S.A. Janjua*,	

	Theoretical modelling of novel indandione-based donor molecules for organic solar cell applications, J. Phys. Chem. Solids (2022) 162, 110508 https://doi.org/10.1016/j.jpcs.2021.110508	3.995/Q2 W
J97	C. C. Nnadiekwe, A. Nada, I. Abdulazeez, M. R. Imam, M.R.S.A. Janjua A. A. Al-Saadi, UV-absorbing benzamide-based dendrimer precursors: synthesis, theoretical calculation, and spectroscopic characterization, New J. Chem. (2022) 46, 75-85 https://doi.org/10.1039/D1NJ04366H	3.591/Q2 W
J96	M.R.S.A. Janjua*, Prediction and Understanding: Quantum Chemical Framework of Transition Metals Enclosed in a $B_{12}N_{12}$ Inorganic Nanocluster for Adsorption and Removal of DDT from the Environment, Inorg. Chem. (2021) 60/14, 10837–10847. https://doi.org/10.1021/acs.inorgchem.1c01760	5.165/Q1 W
J95	M.R.S.A. Janjua*, Theoretical Framework for Encapsulation of Inorganic $B_{12}N_{12}$ Nanoclusters with Alkaline Earth Metals for Efficient Hydrogen Adsorption: A Step Forward toward Hydrogen Storage Materials, Inorg. Chem. (2021) 60 (4), 2816-2828 https://doi.org/10.1021/acs.inorgchem.0c03730	5.165/Q1 W
J94	M.R.S.A. Janjua*, How does bridging core modification alter the photovoltaic characteristics of triphenylamine-based hole transport materials? Theoretical understanding and prediction, Chem. Eur. J. (2021) 27 (12) 4197-4210 https://doi.org/10.1002/chem.202004299	5.236/Q2 W
J93	M.R.S.A. Janjua*, Theoretical Understanding and Role of Guest π-Bridges in Triphenylamine-Based Donor Materials for High-Performance Solar Cells, Energy Fuels, (2021) 35, 15, 12451–12460 https://doi.org/10.1021/acs.energyfuels.1c01625	3.605/Q2 W
J92	M.R.S.A. Janjua*, Quantum Chemical Design of D-π-A Type Donor Materials for Highly Efficient, Photo-stable and Vacuum-processed Organic Solar Cells, Energy Technol., (2021) 9/10, 2100489	3.631/Q3 W
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