



St. Xavier's College

Dr. Camil Bulcke Path, Ranchi

Faculty Profile

Name of Faculty Member	:	Dr. Reman Kumar Singh
Gender	:	Male
Email ID	:	reman_sxc@sxcran.org
Name of Department	:	Department of Chemistry
Designation	:	Assistant Professor
Level of Teaching	:	Undergraduate and Postgraduate
Academic Qualification	:	M.Sc., Ph. D.
Post-Doctoral Research	:	2020-2022 from IIT Bombay
Total Teaching Experience	:	01 Years and 06 Months
UGC NET/SET Qualified	:	Yes

Research Papers Published:

- 1) **Outer-Valence Intermolecular Coulombic Decay in Hydrogen-Bonded Complexes:** Namitha Brijit Bejoy, **RK Singh**, Nitin. K Singh, Balanarayan Pananghat and G. Naresh Patwari. The Journal of Physical Chemistry Letters 14, 5718-5726
- 2) **Dissociation of Endohedrally Encapsulated HCl/HBr in C60 and C70: An Electric Field Perspective:** **RK Singh***, GN Patwari*, The Journal of Physical Chemistry B
- 3) **Unraveling topoisomerase IA gate dynamics in presence of PPEF and its preclinical evaluation against multidrug-resistant pathogens:** Vikas Maurya, Raja Singh, **RK Singh**, Stuti Pandey, Pooja Yadav, Palak Parashar, Rajni Gaind, Kshatresh Dutta Dubey, G Naresh Patwari, Vibha Tandon. Communications Biology volume 6, Article number: 195 (2023).
- 4) **Identification of Allosteric Hotspots regulating the ribosomal RNA-binding by Antibiotic Resistance-Conferring Erm Methyltransferases:** R Bhujbalrao, K

Gavvala, **RK Singh**, J Singh, C Boudier, S Chakrabarti, Journal of Biological Chemistry, 102208

- 5) **Binary Matrix Method to Enumerate, Hierarchically Order, and Structurally Classify Peptide Aggregation:** A Tagad, **RK Singh***, GN Patwari* (Corresponding Author) Journal of Chemical Information and Modeling 62 (6), 1585-1594
- 6) **Molecular Mechanism of Dual Intercalation in Sac7d–DNA Complexation:** RK Singh, A Mukherjee, The Journal of Physical Chemistry B 126 (8), 1682-1690
- 7) **Ultrafast Proton-Transfer Reaction in Phenol–(Ammonia)_n Clusters: An Ab Initio Molecular Dynamics Investigation:** **RK Singh**, R Pant, GN Patwari, The Journal of Physical Chemistry B 126 (7), 1590-1597
- 8) **Role of Sugar Stereochemistry on Structural and Free Energy Landscape of Double-Stranded Nucleic Acid:** A Kumar, **RK Singh**, A Tagad, GN Patwari, bioRxiv, 2020.08. 15.252643
- 9) **Characterization of a Novel Mesophilic CTP-Dependent Riboflavin Kinase and Rational Engineering to Create Its Thermostable Homologues:** Y Kumar, **RK Singh***, AB Hazra*, ChemBioChem 22 (24), 3414-3424
- 10) **Cover Feature: Characterization of a Novel Mesophilic CTP-Dependent Riboflavin Kinase and Rational Engineering to Create Its Thermostable Homologues:** Y Kumar, **RK Singh***, AB Hazra*, ChemBioChem 22 (24), 3359-3359
- 11) **Quantum Transport in DNA Heterostructures: Implications for Nanoelectronics:** SR Patil, H Mohammad, V Chawda, N Sinha, **RK Singh**, J Qi, M P Anantram, ACS Applied Nano Materials 4 (10), 10029-10037
- 12) **Atomistic De-novo Inhibitor Generation-Guided Drug Repurposing for SARS-CoV-2 Spike Protein with Free-Energy Validation by Well-Tempered Metadynamics:** R Chowdhury, V Sai Sreyas Adury, A Vijay, **RK Singh**, A Mukherjee, Chemistry–An Asian Journal 16 (12), 1634-1642
- 13) **Molecular Mechanism of the Intercalation of the SOX-4 Protein into DNA Inducing Bends and Kinks:** RK Singh, A Mukherjee, The Journal of Physical Chemistry B 125 (15), 3752-3762
- 14) **Hierarchy of π -stacking determines the conformational preferences of bis-squaramates:** A Singh, **RK Singh**, GN Patwari, CrystEngComm 23 (31), 5331-5336

- 15) Reply to "**Comment on 'Arresting an Unusual Amide Tautomer Using Divalent Cations'**" SM Kashid, **RK Singh**, H Kwon, JG Seol, YS Kim, A Mukherjee, S Bagchi, The Journal of Physical Chemistry B 125 (1), 479-483
- 16) **Arresting an Unusual Amide Tautomer Using Divalent Cations**: SM Kashid, **RK Singh**, H Kwon, YS Kim, A Mukherjee, S Bagchi, The Journal of Physical Chemistry B 123 (40), 8419-8424
- 17) **Controlling anticancer drug mediated G-quadruplex formation and stabilization by a molecular container**: S Satpathi, **RK Singh**, A Mukherjee, P Hazra, Physical Chemistry Chemical Physics 20 (11), 7808-7818
- 18) **Mechanism of unfolding of human prion protein**: **RK Singh**, NG Chamachi, S Chakrabarty, A Mukherjee, The Journal of Physical Chemistry B 121 (3), 550-564
- 19) **Molecular origin of DNA kinking by transcription factors**: **RK Singh**, WD Sasikala, A Mukherjee, The Journal of Physical Chemistry B 119 (35), 11590-11596
- 20) **Urea induced unfolding dynamics of flavin adenine dinucleotide (FAD): spectroscopic and molecular dynamics simulation studies from femto-second to nanosecond regime**: A Sengupta, **RK Singh**, K Gavvala, RK Koninti, A Mukherjee, P Hazra, The Journal of Physical Chemistry B 118 (7), 1881-1890

Participation in UGC-HRDC Course/FDP/OC/RC:

- 1) GURU-DAKSHATA-FIP-2023 (02-09-2023 to 29-09-2023) organized by HRDC-UGC Ranchi University

Seminar/Conference attended/Paper Presented (National/International):

- 1) Organized the "**Advanced Molecular Dynamics Simulation: A Summer School 2021**" on Molecular dynamic simulation, accelerated technique in MD, force field generation using Charmm module fparam and QM/MM simulation.
- 2) Organized the inhouse "**Molecular Modelling in Chemistry**" workshop on Gaussian, Autodock, MOPAC, molecular modelling, December, 2018, IISER Pune, India.
- 3) Poster Presentation at Rare Event, 2017, "**Mechanism of DNA protein interaction: study of SOX-4-DNA complex formation**", International conference organized by IIT Kanpur".

- 4) Poster Presentation at MCBR, 2015, "**Mechanism of prion protein unfolding**", International conference organized by IIT madras.
- 5) Poster Presentation at Theoretical Chemistry Symposium, 2014, "**Molecular origin of kinking in DNA by transcription factors**", National Conference organized by IISER Pune.
- 6) Poster Presentation at DCCBS, 2014, "**Molecular origin of kinking in DNA by transcription factors**", International conference organized by IIT Kanpur.
- 7) Invited Talk at Inter-IISER chemistry meet, 2015, "**Mechanism of prion protein unfolding**", National conference organized by IISER Bhopal.

[Dr. Reman Kumar Singh]