# Curriculum Vitae

Personal:			
Name Sex	: Dr. Prabhat Kumar Singh : Male		
Date of Birth	: 15 <sup>th</sup> July, 1983		
Nationality	: Indian		

## **Details of Appointments**

Positions held	Institution	From (year)	To (year)	Remarks
Scientific Officer (C)	Bhabha Atomic Research Centre	2006	2008	
Scientific Officer (D)	Bhabha Atomic Research Centre	2008	2012	
Scientific Officer (E)	Bhabha Atomic Research Centre	2012	2016	
Scientific Officer (F)	Bhabha Atomic Research Centre	2016	2022	
Scientific Officer (G)	Bhabha Atomic Research Centre	2022	Till date	
Postdoctoral fellow	University of Pennsylvania, USA	2011	2013	Advisor: Prof. Robin M. Hochstr asser
Assistant Professor	Homi Bhabha National Institute	2016	2022	
Associate Professor	Homi Bhabha National Institute	2022	Till date	

## Academic profile

2011 -2013	<b>Postdoctoral Research</b> ( <i>With Prof. Robin M. Hochstrasser</i> ) University of Pennsylvania, USA <b>Two Dimensional Infrared Spectroscopy</b>
2011 .	PhD Homi Bhabha National Institute Thesis entitled "Studies on the Dynamics of Ultrafast Photoinduced Processes in Condensed Phase using Thioflavin-T and Coumarin as the Probes"
2005-2006	Advanced Courses on Chemical Sciences and Nuclear Sciences (First Rank)

	Bhabha Atomic Research Centre (BARC) Training School Mumbai 400085, India
2003-2005	<b>M.Sc. in Chemistry</b> First Class ( <b>First Rank</b> ) Burdwan University, Burdwan, India
2000-2003	<b>B.Sc. (Honours in Chemistry)</b> First Class Burdwan University, Burdwan, India

#### Awards and/or other recognitions

- 25. Selected for CRS Silver Medal and Award Lecture, 2024
- 24. **Member** of National Committee for IUPAC (2024-2026)
- 23. Selected as Fellow of Maharashtra Academy of Sciences, 2023
- 22. Selected as Fellow of Royal Society of Chemistry (FRSC), 2023
- 21. Selected as **TWAS Young Affiliate** (2023-2028) of World Academy of Sciences, 2023
- 20. Selected as Associate Fellow of Indian National Science Academy (INSA), 2023
- 19. Selected as **Fellow** of Indian Chemical Society (ICS), 2023
- 18. Appeared in the list of top 2 % scientists published by Stanford University in Elsevier,
- 2022

17. Appeared in the list of top 2 % scientists published by Stanford University in Elsevier,2021

- 16. Selected as Member of Global Young Academy (GYA), Halle, Germany, 2020
- 15. Selected for Phys. Chem. Chem. Phys. (PCCP) Emerging Investigator Issue, 2020
- 14. Selected as Young Associate of Maharashtra Academy of Sciences (MASc)-2018
- 13. Selected as Member of National Academy of Science, India (NASI)-2018
- 12. Scientific Planet Society Young Scientist Award-2018
- 11. National Academy of Science, India (NASI) Young Scientist Award 2017
- 10. Selected as Associate of Indian Academy of Sciences (IASc), Bangalore 2017

9. Selected as Member of Indian National Young Academy of Sciences (INYAS-INSA)
- 2017

- 8. Indian Science Congress Association (ISCA) Young Scientist Award-2013
- 7. Department of Atomic Energy (DAE) Young Scientist Award-2013
- 6. Outstanding PhD Thesis Award (HBNI)-2011
- 5. Homi Bhabha Gold Medal 2006

- 4. Dr. Shyama Prasad Mukherjee Fellowship (Awarded by CSIR)- 2005
- 3. Dr. Sumanta Basu Medal- 2005
- 2. Dr. Gouri Kant Mukherjee Gold Medal 2005
- 1. Burdwan University Gold Medal 2005

#### Membership of professional bodies

1. Life member of Indian Society for Radiation and Photochemical Sciences. (ISRAPS,

#### Mumbai)

- 2. Life Member of ISCA, Kolkata, India
- 3. Member, NASI, Allahabad
- 4. Member, INYAS, INSA, NewDelhi, India
- 5. Member, GYA, Halle, Germany
- 6. Life member, MRSI
- 7. Life Member, CRSI
- 8. Life Member, SMC
- 9. Life Member, CRS

### **Research Experience**

17 Years (Total); 12 Years (Postdoctoral Research Experience)

#### **Research Interest**

- Ultrafast Spectroscopy and Sensing Applications of Self-assembled Materials
- Proteins and Protein aggregates
- Fluorescence based Chemosensor and Biosensor
- Femtosecond Time-resolved spectroscopy
- Stimulus-responsive materials
- Dynamics in complex fluids such as ionic liquids and Deep Eutectic Solvents
- Supramolecular Chemistry

#### **Research Accomplishments**

### Peer-reviewed International Journal papers: 129

(h-index: **36**; i-10 index:**79**; total citations: **3160**): Source: Google Scholar Source: <u>www.scholar.google.co.in</u> on 22.03.2024

Webpage: https://scholar.google.co.in/citations?user=tLZ6QKgAAAAJ&hl=en

#### **Summary of Research Work**

Dr. Prabhat Kumar Singh has been instrumental in advancing the field of ultrafast chemical dynamics through the deployment of an array of experimental techniques, most notably femtosecond fluorescence upconversion and two-dimensional vibrational spectroscopy. His scientific contributions extend to self-assembled materials, particularly their practical application for sensing purposes. The following is an elaborative account of his professional journey in research, underscoring his salient accomplishments and expertise.

Dr. Singh has conducted exhaustive research on the ultrafast dynamics of Thioflavin-T, a 'gold standard' marker for amyloid detection. His detailed time-resolved fluorescence studies have, for the first time, illuminated the precise mechanism underlying the fluorescence sensing activity of this prominent amyloid fibril sensor, Thioflavin-T, as documented in his publication in The Journal of Physical Chemistry B (2010, 114, 2541). With the astute application of his scientific acumen, Dr. Singh conceptualized, designed, and synthesized two derivatives of Thioflavin-T. Through this undertaking, he could identify that the rotation around the central carbon-carbon single bond governs the fluorescence sensing activity of Thioflavin-T. This significant finding was published in Chemistry – A European Journal (2010, 16, 9257).



Free Thioflavin-T: Ultrafast twisting Dye bound to fibril: No bond twisting



#### $(k_{rot}=1.7x10^{12}s^{-1})$

In his recent studies, Dr. Singh has unveiled an intriguing phenomenon regarding the fluorescence enhancement observed for Thioflavin-T in insulin fibrils. Despite significant fluorescence amplification, he found that the vast majority of fibril-bound Thioflavin-T undergoes efficient ultrafast conformational relaxation and, as such, does not contribute to the characteristic fluorescence enhancement. His work has critically demonstrated that a substantial proportion of the Thioflavin-T molecules remain bound to the fibril surface, undergoing considerable conformational relaxation. Conversely, the Thioflavin-T molecules which bind to the fibril's channels have been identified as the primary source of the characteristic fluorescence enhancement. This pivotal insight, which further refines our understanding of Thioflavin-T's role in amyloid detection, was published in the Chemical Communications journal (2015, 51, 14042).



In a recent groundbreaking study, Dr. Singh successfully designed a fluorescent sensor for amyloid fibrils operating in the near-infrared region. Significantly, this sensor records the most red-shifted wavelength yet observed for any sensor molecule functioning in this spectral region, specifically for insulin amyloid fibrils. This innovative development marks another notable milestone in Dr. Singh's ongoing contribution to the scientific understanding of amyloid sensing, as reported in the publication in Chemical Communications (2019, 55, 3907).



Dr. Singh has also contributed insightful findings regarding the molecular characteristics of Thioflavin T. He demonstrated that Thioflavin T belongs to the category of ultrafast molecular rotors. Due to its photophysical parameters' extreme sensitivity to viscosity, it can be leveraged to estimate micro-viscosity in micro-heterogeneous environments such as reverse micelles, as documented in The Journal of Physical Chemistry B (2010, 114, 5920; 2009, 113, 8532). Furthermore, he has embarked on an exploration of the effects of supramolecular confinement; specifically the influence of cyclodextrin and its derivatives, on the excited-state dynamics of ultrafast molecular rotors like Thioflavin T and Auramine O. His research in this domain, continues to deepen our understanding of these complex molecular systems.





In an intriguing first, Dr. Singh employed an ultrafast molecular rotor as a fluorescence sensor, enabling him to reveal that the principles of electrostatic interaction can be superseded within a nanoconfined environment. This unexpected deviation occurs when such interactions are collectively assisted by other weak forces, adding a new dimension to our understanding of molecular behavior within such restricted spaces. This groundbreaking discovery was featured in the Chemical Communications journal (2011, 47, 6912).



Dr. Singh has also unveiled the versatile applicability of Thioflavin-T in monitoring subtle structural alterations in natural DNA at pre-melting temperatures, a feat that remains challenging to achieve via other conventional spectroscopic techniques. He further showcased the utility of Thioflavin-T in shedding light on the interactions between DNA and ionic liquids. His pioneering work on the behavior of Thioflavin-T in various confined environments has piqued widespread interest among researchers worldwide. The global scientific community has acknowledged and appreciated his contributions, emphasizing the impact and relevance of his research in the broader context of molecular studies.



In an intriguing sequence of research exploring the formation of supramolecular assemblies between block copolymers and charged surfactant systems, Dr. Singh has shown that through a meticulous selection of the polymer-surfactant supramolecular assembly composition, the chemical reactivity of a solute dissolved in a micro-heterogeneous medium can be fine-tuned, all without altering their chemical identity. This research bears significant implications for the field, underscored by the American Chemical Society's selection of his work as the cover feature for an issue of the Journal of Physical Chemistry B (J. Phys. Chem. B (Letter), 2008, 112, 11447). The spotlight on his work affirms its importance and acknowledges Dr. Singh's ongoing contribution to advancing our understanding of supramolecular assembly interactions.



In a novel study, Dr. Singh unveiled a simple yet innovative strategy for the controlled release of a model drug molecule from a model drug carrier (in this case, a micelle) to an integral component of biological systems, DNA. This process was effectively triggered using biocompatible external stimuli ( $\beta$ -CD). This external stimulus facilitated the quantitative transfer of drug molecules from the micelle to DNA molecules. This groundbreaking research,

which adds a new layer to our understanding of controlled drug delivery systems, was published in The Journal of Physical Chemistry B (2013,117, 10370).



In a subsequent study, Dr. Singh has shown that quantitative sequestration of DNA intercalated model drug molecules can be effectively accomplished through the use of polymer-surfactant supramolecular assemblies. This research has significant implications, particularly for designing treatments for drug overdose cases. His pioneering work in this field, showcasing a potential new avenue for addressing drug-overdose emergencies, was published in The Journal of Physical Chemistry B (2016,120, 4143).



In a recent innovative study, Dr. Singh reported a unique observation of emissive H-aggregates, intriguingly hosted within a charged cyclodextrin cavity. Remarkably, the emission from these aggregates proved extremely sensitive to changes in temperature and the ionic strength of the medium. This property positions these aggregates for potential applications in fields such as optical thermometry, thereby opening up a new realm of possibilities for their practical use. This exciting discovery was highlighted in Chemistry – A European Journal (2016, 22, 7394).



Dr. Singh has ingeniously utilized supramolecular aggregate assembly to construct a simple yet effective fluorescence sensor system. This system is capable of detecting and differentiating between non-metalloproteins and metalloproteins. Interestingly, the system demonstrates distinct response patterns: non-metalloproteins modulate the emission from the supramolecular aggregate assembly in a 'turn-on' and ratiometric fashion, whereas metalloproteins trigger a 'turn-off' response. This stark and contrasting behavior of metalloproteins and non-metalloproteins in the presence of supramolecular aggregate assembly furnishes a compelling and innovative platform for their discrimination. These key findings were published in his article in Chemical Communications (2018, 54, 4537-4540), further contributing to the body of knowledge in this scientific field.



The supramolecular assembly was further harnessed by Dr. Singh to develop a straightforward, ratiometric sensor for basic amino acids, namely lysine, and arginine, using fluorescence spectroscopy. He also demonstrated the successful differentiation of these closely related basic amino acids, arginine, and lysine, by analyzing the fluorescence response pattern using principal component analysis. This approach employs a recognition pattern strategy, further demonstrating the versatility and practical application of supramolecular assemblies in the field of sensor technology.



Constructing "turn-on" fluorescent probes for Heparin, a commonly used anticoagulant in clinical settings, is an area of great interest but poses significant challenges. Recently, Dr. Singh has made a breakthrough in this field by developing a "turn-on" fluorescence sensor for Heparin. This sensor offers several notable advantages. Firstly, it emits in the red region, which is advantageous for biological applications. Secondly, it enables dual sensing capabilities, permitting detection via both fluorimetry and colorimetry. Most significantly, it is constructed from an inexpensive, commercially available dye molecule, which makes it an economical choice. Furthermore, Dr. Singh demonstrated that the novel Thioflavin-T aggregate emission could be used to probe the interaction between Heparin and its only clinically approved antidote, Protamine. This significant development, published in ACS Applied Materials & Interfaces (Letter, 2016, 8, 31505), is expected to leave a considerable imprint on the Heparin sensing field.



In a recent advancement, Dr. Singh has successfully built upon his previous work to develop a dual "turn-on" fluorescence and colorimetry-based "ratiometric" sensor for Heparin. This new sensor is grounded in the J-aggregate assembly of a cyanine-based dye, enabling the naked-eye detection of Heparin, a breakthrough in the field. This significant development, which enhances the accessibility and practicality of Heparin detection, was documented in Sensors and Actuators B: Chemical (2019, 278, DOI: 10.1016/j.snb.2019.127089).



In a recent series of studies, Dr. Singh critically evaluated the performance of a newly proposed amyloid marker, Auramine O. His investigations revealed that Auramine O significantly interacts with the native form of protein (serum albumin). As such, his work underscores the need for careful use of Auramine O as an amyloid marker due to these interactions. This cautionary advice, grounded in a robust scientific examination, was published in The Journal of Physical Chemistry B (2016, 120, 10496-10507).



Dr. Singh has also skillfully harnessed the phenomenon of aggregation-induced emission in molecular rotors to create the first fluorescence "turn-on" sensor for the Perrhenate anion. Notably, Perrhenate serves as a non-radioactive surrogate for the hazardous pertechnetate anion. This innovative development showcases Dr. Singh's unique ability to leverage fundamental scientific phenomena to address real-world challenges. The results of these significant investigations were published in Sensors & Actuators: B. Chemical (2018, 277, 205) and Chemistry - A European Journal (2019, 25, 2035).



Recently, Dr. Singh has pioneered the development of a fluorescence "turn-on" sensor for the serum albumin protein in human serum and urine samples. Notably, this sensor registers the highest fluorescence enhancement in the near-infrared (NIR) region, as documented in his work published in Chemistry Communications (2018, 54, 8383-8386). Motivated by these significant results, Dr. Singh is spearheading the development of a table-top device intended for clinical applications. The ultimate goal is to bring this highly sensitive and efficient detection method out of the research lab and into everyday clinical use, demonstrating his commitment to translating basic scientific discoveries into practical healthcare solutions.



Dr. Singh has recently made another significant contribution to the field by developing a fluorescence "turn-on" sensor for beta-lactoglobulin, a common milk allergen. Notably, this is the first time a fluorescence-based sensor has been developed for this particular milk allergen. This development not only enhances our ability to detect beta-lactoglobulin but also presents potential advancements in ensuring food safety for individuals with milk allergies. This notable work was published in Sensors and Actuators B: Chemical (2021, 327, 128864).



In a recent significant achievement, Dr. Singh developed a technologically advantageous ratiometric sensor for Protamine. Protamine is the sole clinically approved antidote for Heparin and is commonly utilized in anticoagulation therapy. The development of a sensor for this vital clinical substance not only represents a scientific breakthrough but also holds the potential to enhance patient safety and treatment efficacy in clinical settings. This remarkable contribution was detailed in Sensors and Actuators B: Chemical (2020, 303, 127182).



Dr. Singh recently made another remarkable advancement by developing a supramolecularbased ratiometric sensor for ATP, an important bio-analyte. The significance and potential impact of this research was recognized by the Journal of Material Chemistry B, which selected his work as a HOT ARTICLE, highlighting its scientific merit and impact on the field. This significant development was published in the Journal of Materials Chemistry B (2020, 8, 1182-1190). This work is a testament to Dr. Singh's continued contributions to advancing our understanding and analytical capabilities in biochemical processes.



In recent years, Dr. Singh has ventured into the field of ultrafast transient infrared spectroscopy. During his research tenure abroad, he engaged with state-of-the-art 2D IR spectroscopy, gaining invaluable insights and experience. Upon his return to India, Dr. Singh has taken the initiative to apply this expertise locally. He has actively contributed to the indigenous development of a state-of-the-art time-resolved technique, the Two-Dimensional Infrared (2DIR) spectrometer, at the Radiation and Photochemistry Division, BARC. Remarkably, this is the first spectrometer of its kind in India, representing a significant technological advancement for the country's research capabilities in this field. Through these endeavors, Dr. Singh demonstrates not only his dedication to advancing scientific knowledge but also his commitment to fostering the growth of home-grown scientific infrastructure and capabilities.





(2D-IR spectrometer at BARC)

Articles of Dr. Prabhat Kumar Singh highlighted on the cover page of the Journals

