Curriculum Vitae

Dr. Shubhra Ghosh Dastidar
Professor
In-Charge, Division of
Bioinformatics

Bose Institute
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Research Profile: A Computational Biologist, experienced in probing and providing structural and dynamical insights into the fundamental processes in biology using atomistic molecular modeling and simulations with the applications of High Performance Computing. Contributed to the several areas of Biophysical Chemistry and Structural Biology, e.g. protein folding and aggregation, protein-protein and protein-ligand interactions, structure refinement, solvation, membrane properties etc. Bcl2 family, microtubule dynamics, Kinases are the primary areas of focus, which are promising areas of cancer therapeutics. Recent achievements have provided mechanistic insights into of the role of flexibility to modulate protein-protein interactions and have high implications for the benefit of the society, e.g. applications in designing novel therapeutics.

Full time employment:
July 2015-present: Professor
July 2015 - Present: Associate Professor, Bose Institute
Jan 2011- Jun 2015: Assistant Professor, Bose Institute

Education:
- Ph.D. (2006), Chemistry, University of Calcutta, India.
- M. Sc. (2000), Chemistry (Physical)[†], University of Calcutta, India
- B. Sc. (1998), Chemistry, University of Calcutta, India

❖ CSIR-NET (2000) and GATE (2000) qualified

Experience as research fellow
Postdoctoral:
- Aug 2007- Dec 2010: Bioinformatics Institute, Singapore [Advisor: Chandra Verma]
- Jan 2007- Jun 2007: Univ. of Texas, (Galveston), USA [Advisor: Catherine Schein]
- Sep 2005- Dec 2006: Univ. of California (Davis), USA [Advisor: Yong Duan]

Doctoral:
- Oct 2002- Sep 2005: Univ. of Calcutta, India [Supervisor: Chaitali Mukhopadhyay]
- Aug 2000- Oct 2002: I.A.C.S., Kolkata, India [Supervisor: Debashis Mukherjee]

Research supervising experience:
No. of Ph.D. Students submitted thesis/degree awarded: 4
Currently supervising PhD students: 4
No. of summer trainees supervised: 10-12

Teaching experience:

2011-present
- Teaching and coordinating the MSc and PhD courses at Bose Institute for more than 10
- Lectures on Bioinformatics in the Masters course in Biochemistry, University of Calcutta
- Lectures in the Bioinformatics courses in MSc Biochemistry of University of Calcutta and MSc Microbiology in Bidhannagar College
- Lectures in the masters course at Ramakrishna Mission Vivekananda Educational and Research Institute (RKMVERI)

2004-2010

- Lectures, Nanyang Technology University, Singapore; Course title: 'Post graduate in Bioinformatics' (2009)
- Lectures, Jadavpur University, India; Course title: 'Post Graduate diploma in Bioinformatics'

Research grants:

- PI, Funding agency: SERB, duration- 2016-2019, Amount: 30 Lakh (Complete)
- PI, Funding agency: DBT, duration 2012-2015, Amount 64 Lakh (complete)
- PI and coordinator, Bioinformatics Centre and NNP project funded by DBT, is under processing at DBT

Fellowships/awards:

- Sadhan Bose Memorial award : 2000

Membership:

- Indian Biophysical Society
- Society of Biological Chemists, EC member of Kolkata chapter
- American chemical Society (in past)

Administrative experience:

- In-charge, Division of Bioinformatics, Bose Institute, 2019 onwards
- Has been in-charge (temporary time) of Bioinformatics Centre, Bose Institute (pre-2019)
- Member of several academic/administrative committees of Bose Institute, including: Library, Internet, IT and cyber security, Unified academic affairs, Press and Information, Building management system etc.
- Members of staff selection committees in Bose Institute several times

Roles and external experts:

- Member of syllabus design committee and Moderator of examiner, Brainware University
- MSc Biotech examinations, Visva Bharati University
- MSc Biochemistry Examination, University of Calcutta
- Design of syllabus of Post graduate course in Computational Biology, Brainware University
- Ph.D. student selection committee, Department of Chemistry, IIEST
- 'JRF to SRF promotion' assessment committee, Department of Chemistry, University of Calcutta
- Participated as examiner at the Kolkata centre of national level examination BINC in 2012
- Served as external observer at the Guwahati centre of BINC examination in 2013

Organized conferences/seminars:

(i) As a secretary, organized an International level Conference on Informatics and Integrative Biology -2011

(ii) As a committee member, organized International Conference on Informatics and Integrative Biology-2014, an event of the silver jubilee celebration of Bioinformatics Centre of Bose Institute

(iii) Organized one day seminar on high performance computing to spread the awareness on GPU-computing in 2013

(iv) Arranged one day workshop on MD simulation and data analysis in 2013

(v) As a committee member and treasurer, organized INPEC-2017, as a part of the centenary celebration of Bose Institute

(vi) Organizing BIC webinar series since September 2020; organized 10 events so far

Curriculum Vitae

Publications:

1. De A, Maity A, Mazumder M, Mondal B, Mukherjee A, Ghosh S, Ray P, Polley S, **Ghosh Dastidar S**, Basu D., **Plant Sci. 2021**, 309:110953, *Overexpression of LYK4, a lysin motif receptor with non-functional kinase domain, enhances tolerance to Alternaria brassicicola and increases trichome density in Brassica juncea*.
2. Paul D, Basu D, **Ghosh Dastidar S**., **J Mol Model. 2021**;27(5):128. *Multi-conformation representation of Mpro identifies promising candidates for drug repurposing against COVID-19.*
3. Sinha S, **Ghosh Dastidar S.**, **Biochemistry 2020**; 59(45):4353-4366. *Shifting Polar Residues Across Primary Sequence Frames of Transmembrane Domains Calibrates Membrane Permeation Thermodynamics.*
4. Bhattacharyya R, Dhar J, **Ghosh Dastidar S**, Chakrabarti P, Weiss MS., **IUCrJ. 2020**;7(Pt 5):825-834.' *The susceptibility of disulfide bonds towards radiation damage may be explained by S···O interactions.*
5. Shohan MUS, Sinha S, Nabila FH, **Ghosh Dastidar S**, Seraj ZI. ***Front Plant Sci. 2019*** Nov 4;10:1420. *HKT1;5 Transporter Gene Expression and Association of Amino Acid Substitutions With Salt Tolerance Across Rice Genotypes*.
6. Meher G, Sinha S, Pattnaik GP, **Ghosh Dastidar S***, Chakraborty H.*, **J *Phys Chem B. 2019*** Aug 22;123(33):7113-7122. *Cholesterol Modulates Membrane Properties and the Interaction of gp41 Fusion Peptide To Promote Membrane Fusion.*
7. Maity A, Sinha S, **Ghosh Dastidar S**., **Chem Phys Lipids. 2019** ;218:112-124., *Dissecting the thermodynamic contributions of the charged residues in the membrane anchoring of Bcl-xl C-terminal domain.*
8. Majumdar S, Basu D, **Ghosh Dastidar S**., **J Chem Inf Model. 2019**;59(5):2274-2286. , *Conformational States of E7010 Is Complemented by Microclusters of Water Inside the α,β-Tubulin Core.*
9. Chakraborty J, Priya P, **Ghosh Dastidar S**, Das S., **Plant Sci. 2018**;276:111-133., *Physical interaction between nuclear accumulated CC-NB-ARC-LRR protein and WRKY64 promotes EDS1 dependent Fusarium wilt resistance in chickpea.*
10. Maity A, Majumdar S, **Ghosh Dastidar S**., **Comput Biol Chem. 2018** Dec;77:17-27. , Flexibility enables to discriminate between ligands: Lessons from structural ensembles of Bcl-xl and Mcl-1.
11. Sinha S, Maity A, **Ghosh Dastidar S., J Chem Inf Model. 2018** Feb 26;58(2):370-382. *, BIM Binding Remotely Regulates BAX Activation: Insights from the Free Energy Landscapes.,*
12. Basak P, Maitra-Majee S, Das JK, Mukherjee A, **Ghosh Dastidar S**, Pal Choudhury P, Lahiri Majumder A., **PLoS One. 2017** Sep 26;12(9):e0185351. , *An evolutionary analysis identifies a conserved pentapeptide stretch containing the two essential lysine residues for rice L-myo-inositol 1-phosphate synthase catalytic activity.*
13. Priya P, Maity A, **Ghosh Dastidar S**., **Proteins Struc Func Bioinf 2017** ;85(8):1567-1579. , *The long unstructured region of Bcl-xl modulates its structural dynamics.*
14. Majumdar S, **Ghosh Dastidar S**., **J Phys Chem B. 2017**;121(1):118-128., *Ligand Binding Swaps between Soft Internal Modes of α,β-Tubulin and Alters Its Accessible Conformational Space.*
15. Maity A, Sinha S, Ganguly D, **Ghosh Dastidar S., Phys Chem Chem Phys. 2016** ;18(34):24095-105. *C-terminal tail insertion of Bcl-xL in membrane occurs via partial unfolding and refolding cycle associating microsolvation.*
16. Majumdar S, Maiti S, **Ghosh Dastidar S, Biochemistry 2016**; 55, 335-47. *Dynamic and Static Water Molecules Complement the TN16 Conformational Heterogeneity inside the Tubulin Cavity.*
17. Sinha A, Ray A, Ganguly S, **Ghosh Dastidar S**, Sarkar S., **Biol Direct. 2015**;10(1):56. *Variation in the ribosome interacting loop of the Sec61α from Giardia lamblia.*

18. Bhar K, Maity A, Ghosh A, Das T, **Ghosh Dastidar S**, Siddhanta A., **Protein J. 2015** Apr;34(2):158-67., *Phosphorylation of Leghemoglobin at S45 is Most Effective to Disrupt the Molecular Environment of Its Oxygen Binding Pocket*
19. Priya P, Maity A, Majumdar S, **Ghosh Dastidar S.**, **J Mol Graph Model. 2015**;59:1-13. *Interactions between Bcl-xl and its inhibitors: Insights into ligand design from molecular dynamics simulation.*
20. Maity A, Majumdar S, Priya P, De P, Saha S, **Ghosh Dastidar S**, **J Biomol Struct Dyn. 2015**;33(2):298-321 *Adaptability in protein structures: Structural dynamics and implications in ligand design (Review)*
21. Maity A, Yadav S, Verma CS, **Ghosh Dastidar S**, **PLoS One (2013**) 8, e76837. *Dynamics of Bcl-xl in Water and Membrane: Molecular Simulations*
22. Sengupta A, Sarkar A, Priya P, **Dastidar SG**, Das S, **PLoS One 2013**, 8, e78249. *New Insight to Structure-Function Relationship of GalNAc Mediated Primary Interaction between Insecticidal Cry1Ac Toxin and HaALP Receptor of Helicoverpa armigeraí.*
23. Chakraborti S, Chakravarty D, Gupta S, Chatterji BP, Dhar G, Poddar A, Panda D, Chakrabarti P, Ghosh **Dastidar S*** and Bhattacharyya B*, **Biochemistry 2012,** 51,7 138*, Discrimination of Ligands with Different Flexibilities Resulting from the Plasticity of the Binding Site in Tubuli*n
24. **Dastidar SG**, Lane DP, Verma CS, **Cell Cycle 2012**, 11: 2239-47, *Why is F19Ap53 unable to bind MDM2? Simulations suggest crack propagation modulates binding*
25. C. J. Brown[£], **S. G. Dastidar**[£], S. T. Quah, A. Lim, B. Chia, C. S. Verma. **PLoS One 2011**, 6, e24122, *C-Terminal Substitution of MDM2 Interacting Peptides Modulates Binding Affinity by Distinctive Mechanisms*
26. G. Fuentes, **S. G. Dastidar**, A. Madhumalar, C. S. Verma, **Drug Dev. Res. 2011,** 72, 26**,** *Role of protein flexibility in the Discovery of New Drugs* (Review Article)
27. S. G. Dastidar, D. Raghunathan, J. Nicholson, T. R. Hupp, D. P. Lane, C. S. Verma, **Cell Cycle 2011,** 10, 82, *Chemical States of the N-terminal "lid" of MDM2 regulate p53 binding*
28. N. J. Bruce[£], D. Chen[£], **S. G. Dastidar**[£], G. E. Marks, C. H. Schein, R. A. Bryce, **Peptides 2010** 31, 2100**,** *Molecular dynamics simulations of Aβ fibril interactions with β-sheet breaker peptides*
29. **S. G. Dastidar**, A. Madhumalar, G. Fuentes, D. P. Lane, C. S. Verma, **Theor. Chem. Acc. 2010,** 125, 621**,** *Forces mediating protein-protein interactions: a computational study of p53 "approaching" MDM2*
30. C. J. Brown, **S. G. Dastidar**, H. See, D. W. Comber, M. Ortiz-Lombardía, C. S. Verma, D. P. Lane, **J. Mol. Biol 2010,** 235, 871, *Rational Design and biophysical characterization of Thioredoxin-based aptamers: Insights into peptide grafting*
31. **S. G. Dastidar**, D. P. Lane, C. S. Verma, **BMC Bioinformatics 2009**, 10 (Suppl 15):S6, *Modulation of p53 binding to MDM2: computational studies reveal important roles of Tyr100*
32. S. Liu, L. Zhou, **S. G. Dastidar,** C. Verma, J. Li, D. Tan and R. Beuerman, **J. Peptide Sci 2009,** 15, 95**,** *Effect of structural parameters of peptides on dimer formation and highly oxidized side products in the oxidation of thiols of linear analogs of human β-defensins-3 by dimethyl sulfoxide.*
33. **S. G. Dastidar**, D. P. Lane and C. S. Verma, **J. Am. Chem. Soc. 2008**, 130, 13514, *Multiple conformation give rise to similar binding affinities: Molecular simulation of p53-MDM2.* ***This article is also archived in a JACS special issue for its excellence***
34. H. Liu, **S. G. Dastidar**, H. Lei, W. Zhang, M. C. Lee, and Y. Duan, **Methods in Molecular Biology book series**. **2008**, 443, 258, Humana Press, *Conformational changes in protein functions,* in Molecular Modeling of Proteins.
35. G. Ping, **S. G. Dastidar** and Y. Duan, **J. Chem. Phys. 2007,** 126, 045108**,** *Statistical Properties and Kinetics of End-end Contact Formation of Unfolded Polypeptides: A Systematic Molecular Dynamics Study.*

36. H. Lei[£], **S. G. Dastidar**[£] and Y. Duan, **J. Phys. Chem. B 2006,** 110*,* 22001**,** *Folding Transition state and Denatured state ensemble of FSD-1 from folding and unfolding simulation*.
37. **S. G. Dastidar** and C. Mukhopadhyay, **Phys. Rev. E. 2005,** 72, 051928**,** *Unfolding dynamics of the protein ubiquitin: Insight from simulation*
38. S. Mondal, **S. G. Dastidar** and C. Mukhopadhyay, **J. Surface Sci. and Tech. 2004,** 20, 237**,** *Effect of different local anesthetics on a phospholipid bilayer: A comparative molecular dynamics simulation study with anesthetic molecules of different strengths of action*
39. **S. G. Dastidar** and C. Mukhopadhyay, **Phys Rev. E 2004,** 70, 061901**,** *Anomalous behavior of water around sodium dodecyl sulphate micelles*
40. **S. G. Dastidar** and C. Mukhopadhyay, **Phys. Rev. E. 2003,** 68, 021921**,** *Structure, dynamics, and energetics of water at the surface of a small globular protein: A molecular dynamics simulation*

[£]***Equal contribution / Joint first author***

Oral presentations and hands-on workshops: in India and abroad

1. March 2011: Talk and hands-on session in the workshop at Kalyani University, India
2. June 2011: Talk in 'Albany 2011: the 17th conversation' at SUNY, Albany, USA
3. August 2011: Talk in the workshop at North Eastern Hill University, India
4. November 2011: Talk and Hand's-on session in the workshop at Kalyani University, India
5. February 2012: Oral presentation in BBCon2012 organized by North Bengal University, India
6. March 2012: 2 days visit and talk at Nanyang Tech University, Singapore
7. March 2012: One day visit and talk at Bioinformatics centre (A*STAR), Singapore
8. December 2012: Oral presentation at Computer-Aided Drug Design, 3-7 December 2012, UiTMPuncakAlam Campus, Kuala Lumpur, Malaysia
9. December 2012: One day visit and talk at Chulalongkorn University, Bangkok, Thailand
10. November 2013: Talk and hands-on session in the workshop "Modeling and Drug Designing" to be held during 18-22nd November,2013 held in Kalyani University, India
11. Oral presentation National Workshop on GPU Programming and Applications (GPA3-2014), 12th - 14th September, 2014, IIT Guwahati, India
12. National Science day lecture at District science centre, Purulia, India
13. Chairing session at the Workshop on electronic structure, atomistic and statistical modelling in Chemistry, Materials and Life Sciences, Oct 20-22, 2014 at IACS, Kolkata, India
14. Oral presentation in the workshop entitled 'Modern Methods in Computing Biology:A Brainstorming Workshop' held at Bioinformatics Institute (A*STAR), Singapore during March 2015
15. 'National Seminar and Workshop on Bioinformatics', North Bengal University, March 2015
16. 'Molecular Graphics and Modelling Society' (MGMS) conference, Singapore (A*STAR), Singapore, September 2015
17. CMTPI international conference at Goa, during Oct 27-30, 2017
18. Talk and hands-on sessions at the workshop 'Protein Sequence to Structure', held during April 15-17, 2018 at University of Dhaka.
19. Seminar on seminar is "Microbial Diversity and Environment-a Bioinformatics Perspective". North Bengal University, March 2019
20. National Workshop, Bioinformatics Infrastructural facility, University of Kalyani, March 2019
21. Seminar organized by Society of Biological Chemists, Kolkata chapter, CSIR-IICB, Kolkata 2019

22. Invited talk at the conference cum brainstorming session entitled 'National Frontier of Science' at Jaipur during Nov 6-8, 2019, organized by Indian National Young Academy of Science with the support of the Office of the Principal Scientific Advisor (PSA) to the Govt. of India.
23. Talk at Belur Vidyamandir, February 2020
24. Talk at the seminar on "Symposium: Drug-on: a battle tale of two creatures – microbes and humans" organized by JIS Institute of Advanced Studies and Research Kolkata on February 29, 2020
25. Presentation at the webinar organized by Indna LifeSciences as a part of the celebration of World DNA day, April 2020
26. Webinar Organized by University of Kalyani, West Bengal on June 11, 2020
27. Webinar organized by Asustosh College and Moulana Azad college of University of Calcutta, August 2020
28. Webinar organized by Barasat College under West Bengal state university, September 8, 2020
29. webinar on the theme "From Biology to Omics" organized by ACTREC, Mumbai, during March 10-12, 2021
30. Keynote at the workshop organized by JIS institute of Advanced studies and research, Kolkata, May 24, 2021

Pre-2011

i. IHPC Computational Science and Engineering Seminar, November **2010** Fusionopolis, Singapore, Title: Simulating the dynamics of biological systems in computer: Advantages and challenges

ii. The International Conference on Bioinformatics (INCOB-2009), September **2009**, Singapore Title: *Modulation of p53 binding to MDM2: computational studies reveal important roles of Tyr100*

iii. Workshop on Computational System Biology approaches to analysis of Genome Complexity and Regulatory Gene networks, November **2008**, Singapore. Title: *Thermodynamic insights based on atomistic computer simulations reveal an intricate coupling between enthalpy and entropy*

iv. TACC conference, September **2008**, Shanghai, China, Title: *Interrupting the MDM2-p53 interface with high affinity: Computational studies*

v. Workshop on Advanced Computing for the Biomedical Sciences, January **2008**, Genome Institute of Singapore. Title: *Challenges in Biomolecular 3D Structural Simulations: the Petascale and Beyond*

Poster presentations:

1. *Mutual modulations of protein-protein interactions: pictures from molecular simulations of MDM2-p53,* S. G. Dastidar, D. P. Lane, C. S. Verma, International Conference on Physics Biology Interface, December **2009**, Kolkata, India
2. *The enthalpy-entropy drama of a peptide: simulation studies of p53,* S. G. Dastidar, D. P. Lane, C. S. Verma, Joint 5th Structural biology and Functional genomics and 1st Biological Physics International Conference, December **2008,** Singapore.
3. *Understanding p53 interactions for therapy,* A. Madhumalar, J. T. Leonard, S. G. Dastidar, H. J. Lee, M. Hui, C. S. Verma, A*STAR Scientific Conference, November **2008**, Singapore.
4. *Molecular dynamics simulations of the interaction of amyloid β-fibrils with peptides that inhibit aggregation*, S. G. Dastidar, D. Chen, G. E. Marks, R. A. Bryce, and C. H. Schein, Structural Biology Symposium, May **2007**, University of Texas Medical Branch, USA
5. *Thermal Unfolding of Ubiquitin in explicit water*, S. G. Dastidar and C. Mukhopadhyay , CRSI symposium, February **2005**, Kolkata, India.
6. *Dynamics, structural characteristics and energetics at the micelle-solvent interface,* S. G. Dastidar and C. Mukhopadhyay, TACC conference, February **2004**, Gyengju, Korea.

7. *Structural properties and slow dynamics of water at the protein-water and the micelle-water interface: A comparative study using molecular dynamics simulation*, S. G. Dastidar and C. Mukhopadhyay *,* NCBS Symposium on Molecules Machines and Network, January **2004**, Bangalore, India.

Workshops attended:

1. Biomolecular solvation modeling with APBS and PDB2PQR conducted by Prof. Nathan Baker, Bioinformatics Institute, Singapore, April **2009**
2. *Methods and Applications of Hybrid QM/MM Simulations to Biomolecular Systems* conducted by Martin Field and Troy Wyemore, Bioinformatics Institute, Singapore, September **2008**

Social activities (scientific):

- Has been an environmental activist, particularly focusing in the **water conservation**
- Given lecture on "Water Conservation and its benefits" at Bethune School, Kolkata on Aug 30, 2019 as a part of their program of "Nirmal Vidyalaya Saptaha" **Bethune Collegiate School**
- Discussed various aspects of 'Water conservation' on **All India Radio**, on Sep 5, 2019
- Invited judge, at the Science exhibition at La Martiniere for Boys, Kolkata on July 26, 2021

Miscellaneous:

Year of Birth : 1976
Gender: Male
Permanent home address: Panna Jheel 4, Barasat, Kolkata 700125, India

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