CURRICULUM VITAE

Name: SRIJEETA TALUKDER

Current position: Assistant Professor

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Date of Birth : 31/07/1987

Nationality : Indian

Sex : Female

Marital status : Married

ACADEMIC QUALIFICATIONS

PhD	PhD in Chemistry (physical), degree has been awarded on **2nd March 2016**. Department of Chemistry, University of Calcutta. Thesis title "**A Stochastic Approach Towards The Study Of Kinetics In Some Biological And Chemical Systems**".
POST GRADUATATION	M.Sc.(Chemistry, Physical special), Presidency College Kolkata (University of Calcutta), India. Year of passing: 2010 Percentage of marks: 72.4
GRADUATATION	B.Sc.(Chemistry Honours), Bidhannagar Government College, University of Calcutta, Kolkata, India. Year of passing: 2008 Percentage of marks: 59.0

HS	Year of passing: 2005 Percentage of marks: 71.4
Madhyamik	Year of passing: 2003 Percentage of marks: 83.37

PROJECT

- Start-Up grant from SERB (from October, 2022). Title: “Soft-Computing based approach towards the study of controlled quantum dynamics on ab initio surface.”

EXPERIENCE

- Assistant Professor in Chemistry at Adamas University from 14/09/2021.
- Assistant Professor in Chemistry at Shri Ramasamy Memorial University Sikkim from 15/07/2019 to 01/10/2020.
- National Post-doctoral Fellow (SERB, India) in Indian Association for the Cultivation of Science from 04/09/2017-12/07/2019.
- Research Associate-I in Indian Association for the Cultivation of Science, from 01/07/2016 to 01/09/2017.
- I am working as Guest lecturer for postgraduate teaching at APC College, West Bengal, since August 2014.
- I have also experience in undergraduate teaching (have worked as Guest Lecturer in Mrinalini Dutta Mahabidyapith, Birati from September 2015-February 2017).

RESEARCH INTEREST

- Theoretical and computational chemistry.
- Ab initio surface generation. Non Adiabatic calculation.
- Quantum dynamics.
- Optimal control theory. We use stochastic optimization to design optimal laser field to control quantum dynamical phenomena.
- Nanoclusters. Structures and properties analysis using stochastic optimization algorithm.
- Mapping out reaction path using stochastic optimizer.
- Stochastic simulation algorithms.

SCHOLARSHIPS

Qualified CSIR-UGC **National Eligibility Test (NET)** in Chemical Sciences as Junior Research Fellow held on 21th June 2009 and recipient of research fellowship.

Also qualified GATE on 2010.

COMPUTER PROFICIENCY

- Programming in FORTRAN, C++, Python
- Software: Gaussian, MOLPRO

THESIS SUPERVISOR :

Prof. Pinaki Chaudhury
Department of Chemistry,
University of Calcutta
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PUBLICATIONS

1. Determining the DNA stability parameters for the breathing dynamics of heterogeneous DNA by stochastic optimization. **Srijeeta Talukder**, Pinaki Chaudhury, Ralf Metzler and Suman K. Banik, J Chem. Phys. **135** 165103 (2011).

2. Optimal designing of polychromatic field for maximum dissociation of LiH molecule. Shrabani Sen, **Srijeeta Talukder** and Pinaki Chaudhury, Indian J. Phys. **87** 865 (2013).

3. Selective bond breaking mediated by state specific vibrational excitation in model HOD molecule through optimized femtosecond IR pulse: A simulated annealing based approach. Bhavesh K. Shandilya, Shrabani Sen, Tapas Sahoo, **Srijeeta Talukder**, Pinaki Chaudhury and Satrajit Adhikari, J. Chem Phys. **139** 034310 (2013).

4. Stochastic optimization-based study of dimerization kinetics. **Srijeeta Talukder**, Shrabani Sen, Ralf Metzler, Suman K. Banik and Pinaki Chaudhury, J. Chem. Sci. **125** 1619 (2013).

5. A parallel tempering based study of Coulombic explosion and identification of dissociating fragments in charged noble gas clusters. **Srijeeta Talukder**, Shrabani Sen, Soumya Ganguly Neogi and Pinaki Chaudhury, J. Chem. Phys. **139** 164312 (2013).

6. Coherent destruction of tunneling with optimally designed polychromatic external field. Subhasree Ghosh, **Srijeeta Talukder**, Shrabani Sen and Pinaki Chaudhury, Chem. Phys. **425** 73 (2013).

7. Structural and spectroscopic studies of carbon dioxide clusters: a combined genetic algorithm and DFT based study. Soumya Ganguly Neogi, **Srijeeta Talukder** and Pinaki Chaudhury, Struc. Chem. **25** 909 (2013).

8. A generalized recipe to construct elementary or multi-step reaction paths via a stochastic formulation: Application to the conformational change in noble gas clusters. **Srijeeta Talukder**, Shrabani Sen, Rahul Sharma, Suman K. Banik and Pinaki Chaudhury, Chem. Phys. **431-432** 5 (2014).

9. Breathing dynamics based parameter sensitivity analysis of hetero-polymeric DNA. **Srijeeta Talukder**, Shrabani Sen, Prantik Chakraborti, Ralf Metzler, Suman K Banik and Pinaki Chaudury, J. Chem. Phys. **140** 125101 (2014).

10. Optimized polychromatic field mediated suppression of H-atom tunneling in a coupled symmetric double well : two dimensional malonaldehyde model. Subhasree Ghosh, **Srijeeta Talukder**, Shrabani Sen and Pinaki Chaudhury, Mol. Phys. **113** 3826 (2015).

11. Enhancing the branching ratios in the dissociation channels for $O^{16}O^{16}O^{18}$ molecule by designing optimum laser pulses: A study using stochastic optimization. **Srijeeta Talukder**, Shrabani Sen, Bhavesh K. Shandilya, Rahul Sharma, Pinaki Chaudhury and Satrajit Adhikari, J. Chem. Phys. **143** 144109 (2015).

12. Deciphering parameter sensitivity in the BvgAS signal transduction. Tarunendu Mapder, **Srijeeta Talukder**, Sudip Chattopadhyay and Suman K Banik, Plos One, DOI:10.1371/journal.pone.0147281 (2016).

13. Selective bond dissociation of HOD molecule by optimally designed polychromatic IR+UV pulse: a genetic-algorithm-based study. **Srijeeta Talukder**, Pinaki Chaudhury and Satrajit Adhikari. Mol. Phys. **115** 1786 (2017).

14. An adaptive mutation simulated annealing based investigation on Coulombic explosion and identification of dissociation patterns in $(CO2)_n^{2+}$ clusters. Pulak Naskar, **Srijeeta Talukder** and Pinaki Chaudhury. Phys. Chem. Chem. Phys. **19** 9654 (2017).

15. Simulated Annealing based optimal control over tunneling process through SDWP and Eckart barrier: A momentum basis representation, **Srijeeta Talukder**, Pinaki Chaudhury and Subhasree Ghosh. International Journal of Quantum Chemistry, **117** e25388 (2017).

16. Structural, spectroscopic and thermodynamic aspects of azide-water clusters: an approach using a conjugated prescription of stochastic and quantum chemical methods, Pulak Naskar, Rituparna Roy, **Srijeeta Talukder** and Pinaki Chaudhury, Mol. Phys. **116** 2172 (2018).

17. The effect of stochastic barrier fluctuation on semi-classical transmission probability and Shannon entropy of a symmetric double well potential, Pulak Naskar, **Srijeeta Talukder**, Pinaki Chaudhury and Subhasree Ghosh. International Journal of Quantum Chemistry **118** e25667 (2018).

18. Controlling the isomerisation dynamics of iodide acetonitrile dimer complex by optimally designed electromagnetic field: a wave packet based approach, Pulak Naskar, **Srijeeta Talukder**, Subhasree Ghosh and Pinaki Chaudhury. International Journal of Quantum Chemistry **119** e25927 (2019).

19. A two state model of photo-detachment dynamics driven by an optimally designed polychromatic field: A simulated annealing based optimization, **Srijeeta Talukder**, Dipayan Seal, Pulak Naskar, Pinaki Chaudhury and Subhasree Ghosh. International Journal of Quantum Chemistry **121** e26676 (2021).

20. An Overview on Simulated Annealing Vs Adaptive Mutation Simulated Annealing, **Srijeeta Talukder**, Journal of Sustainable Science and Transformative Research-Reviews & Letters **1** 63 (2022).

21. Mapping Of DNA Base-pair Sequence From Breathing Dynamics Of Hetero-polymeric DNA: A Genetic Algorithm Based Study, **Srijeeta Talukder,** Journal of Chemical Sciences **136** 30 (2024).

22. Energetics and spectroscopic studies of $CNO^-(H_2O)_n$ clusters and the temperature dependencies of the isomers: An approach based on a combined recipe of parallel tempering and quantum chemical methods, Pulak Naskar and **Srijeeta Talukder**, J. Comp. Chem. **45**, 2749 2024

TEACHING EXPERIENCE:

I am acquainted with the undergraduate and postgraduate teaching of Physical Chemistry (I have experiences both in undergraduate and postgraduate teaching). I would like to teach quantum mechanics and thermodynamics in both undergraduate and postgraduate level. However I am able to teach other topics of chemistry too.

I also use to take courses on numerical analysis and programming. Knowing programming is a very important as per as the demand of modern research. I am well versed with programming and would like teach preliminary as well as advance courses of scientific computing.

RESEARCH HIGHLIGHTS:

During my PhD tenure:

In my thesis work the primary aim was to inquire the possibility of using stochastic optimization algorithms in solving the problems of kinetics. There are two gross aspects of studying kinetics. Firstly, by writing rate equations according to the network and then solve

them in order to get the time evolution. Another aspect is to follow reactions at molecular level. In this thesis work both the aspects of kinetics have been addressed.

I have also interest in optimal control theory. Apart from my thesis work I have publications in Quantum dynamics, where the aim was to optimally control a phenomenon (like selective dissociation in HOD and $O^{16}O^{16}O^{18}$, controlling tunneling dynamics) by designing proper electromagnetic radiation.

Recent development and future plans:

Recently I am continuing my research on optimal control theory, where the dynamics will be studied on ab initio potential surface. Now I am working in the project of getting selective bond dissociation in halomethanes like CH_2ClBr. Unlike HOD and $O^{16}O^{16}O^{18}$ it is a three state problem. Previously the problems which were attempted have analytical form of potential energy surface, however this is not the case for CH_2ClBr. We are evaluating the ab initio potential energy surface as well as dipole and transition dipole moment surface for the study. To get proper surface for dynamics we have to go beyond Born-Oppenheimer regime and have to calculate the non-adiabatic coupling terms between the electronic states. Our plan is to study and eventually control the dynamics of this system in the diabetic potential surface. Also controlling photodetachment and photo-dissociation is the another type of quantum control extensively studied by us.

I am also carrying out research on clusters. Structural evaluation and also reaction path are the two major aspect of doing research in this field. Recently I am pursuing theoretical study of adsorption on metal molecular cluster

I have applied or modulated the stochastic optimizers in solving diverse problems where some of them are not commonly treated by this strategy. As a future plan I want to explore the area of research of algorithmic progression based on evolutionary computation or artificial intelligence. Rather I am working on Artificial Neural Network (ANN) recently. We have a plan to make a conjunction of stochastic optimizer with ANN for the construction of potential energy surface and can follow dynamics (Quantum dynamics) on that surface.

REFEREES

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