

# CURRICULUM VITÆ

## Current positions and address for correspondence

**Name:** Dr Amit S Tiwary

**Designation:** Associate Professor

**Specialization:** Organic Chemistry

**Department:** Department of Chemistry

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## Residential Address

434 G. T. Road East End,  
Parbirhata, Post- Sripally,  
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## Teaching Experience

*Joined the college as Lecturer in the year 2002, promoted to Senior Lecturer in 2008 later designated as Assistant Professor and finally promoted to Associate Professor in 2016. Has been teaching Organic Chemistry for almost 21 years.*

## Current Research Interests

*Graph theoretical and computational study of charge transfer complexes and organic reaction mechanisms.*

## Educational Qualification

Name of the Degree	Name of the University/Board	Year	Specific Subject Area
Ph. D. in Chemistry	The University of Burdwan	2009	Theoretical Computational Chemistry  [Title of the Ph.D Thesis: "APPLICATION OF GRAPH THEORY AND DENSITY FUNCTIONAL THEORY IN THE STUDY OF SOME PHYSICO-CHEMICAL PROBLEMS"]
M.Sc. (Chemistry)	The University of Burdwan	2000	Organic Chemistry
B.Sc.	The University of Burdwan	1998	Chemistry Honours
Higher Secondary	WBCHSE	1995	
ICSE	CISCE, New Delhi	1993	

## Publications (Research Articles)

- 1 Study of charge transfer transition in benzene-ICl complex in gas phase and in CCl<sub>4</sub> medium by ab initio and TDDFT methods  
**Amit S. Tiwary**, Partha Sarathi Sengupta and Asok K. Mukherjee, *Chem. Phys. Lett.* **433** (2007) 427-431. Impact Factor-2.029, Citations-16, Reads-95
- 2 Modeling the Ground State Geometry and Estimating the Charge Transfer Transition Energy of the Toluene-ICl Molecular Complex by Ab Initio and DFT Methods  
**Amit S. Tiwary**, Partha Sarathi Sengupta and Asok K. Mukherjee, *J. Theor. Comput. Chem.(JTCC)* **7** (2008) 331-346. Impact Factor- 0.939, Citations-06, Reads-356

- 3 Ab initio and TDDFT study of the structural and spectroscopic properties of buckybowls: Corannulene and two methylcorannulenes  
**Amit S. Tiwary** and Asok K. Mukherjee, *J. Mol. Struct. THEOCHEM*, **859** (2008) 107-112. Impact Factor- 2.011, Citations-29, Reads-50
- 4 Charge transfer interaction of 4-acetamidophenol (paracetamol) with 2,3-dichloro-1,4-naphthoquinone: A study in aqueous ethanol medium by UV-vis spectroscopic and DFT methods  
Avijit Saha, **Amit S. Tiwary** and Asok K. Mukherjee, *Spectrochim. Acta* **71** (2008) 835-840. Impact Factor- 4.098, Citations-09, Reads-33
- 5 Construction and studies of a new class of reciprocal trees: interknitting of the Pascal's Triangle  
**Amit S. Tiwary**, Bholanath Mandal and Asok K. Mukherjee, *Mol. Phys.* **106** (2008) 1813-182. Impact Factor- 1.767, Citations-11, Reads-21
- 6 Inductive effect of methyl group in the light of HMO and DFT methods  
**Amit S. Tiwary** and Asok K. Mukherjee, *J. Mol. Struct. THEOCHEM* **867** (2008) 90-94. Impact Factor- 2.011, Citations-02, Reads-29
- 7 Graph theoretical parameters for  $\pi$ -MO calculation of phenols from DFT-calculated energies: Application to charge-transfer complexes  
**Amit S. Tiwary** and Asok K. Mukherjee, *Mol. Phys.* **106** (2008) 2271-2276. Impact Factor- 1.767, Citations-04, Reads-24
- 8 Mechanism of the  $\text{CH}_3\text{NH}_2$  -  $\text{HNO}_2$  reaction: Ab initio DFT/TST study  
**Amit S. Tiwary** and Asok K. Mukherjee, *J. Mol. Struct. THEOCHEM* **909** (2009) 57-65. Impact Factor- 2.011, Citations-11, Reads-52
- 9 Calculation of Charge Transfer Transition Energy of the Mesitylene-ICl Complex by *ab initio* and TDDFT method: Comparison with Some Other Methylbenzene-ICl Complexes  
**Amit S. Tiwary** and Asok K. Mukherjee, *Mol. Phys.* **107** (2009) 2063-2070. Impact Factor- 1.767, Citations-04, Reads-41
- 10 Graph-theoretical parameters of  $\pi$ -MO calculation of a series of aromatic amines in the light of DFT theory: comparison with experimental CT transition energies  
**Amit S. Tiwary**, Nipmanjari Deb and Asok K. Mukherjee, *Mol. Phys.* **108** (2009) 1599-1605. Impact Factor- 1.767, Citations-18, Reads-92
- 11 Calculation of the Kirkwood-Frohlich correlation factor and dielectric constant of methanol using a statistical model and density functional theory  
Nipmanjari Deb, **Amit S. Tiwary** and Asok K. Mukherjee, *Mol. Phys.* **108** (2010) 1907-1917. Impact Factor- 1.767, Citations-08, Reads-252

- 12 Inductive effect of methyl group in a series of methylated indoles: A graph theoretical analysis in the light of density functional theory and correlation with experimental CT transition energies  
**Amit S. Tiwary** and Asok K. Mukherjee, *Journal of Chemical Sciences*. **125** (2013) 905-912. Impact Factor-1.406, Citations-04, Reads-160
- 13 Origin of degeneracy in the HMO eigenspectra of some  $\pi$ -systems with Abelian point groups  
**Amit S. Tiwary**, *5 FOCUS* (2014) 80-92.
- 14 Performance of the M06 family of functionals in prediction of the charge transfer transition energies of the naphthalene–TCNE and pyrene–TCNE molecular complexes  
**Amit S. Tiwary** and Asok K. Mukherjee, *Chem. Phys. Lett.* **610-611** (2014) 19-22. Impact Factor-2.029, Citations-09, Reads-38
- 15 Performance of the M06 family of functionals in predicting the charge transfer transition energies of molecular complexes of TCNE with a series of methylated indoles  
**Amit S. Tiwary**, Kakali Datta and Asok K. Mukherjee, *Comput. Theoret. Chem.* **1068** (2015) 123-127. Impact Factor- 1.403, Citations-06, Reads-44
- 16 Nature's Choice of Structures: Fibonacci Sequence  
**Amit S. Tiwary**, *FOCUS*, **7** (2016) 173-180.
- 17 Lucas sequence and Fibonacci triads of graphs for analysis of charge transfer spectra of complexes of a series of methylated indoles  
**Amit S. Tiwary** & Bankim Chandra Ghosh, *J. Indian Chem. Soc.*, **96** (2019) 659-665.
- 18 Prediction of charge transfer transition energies of the molecular complexes of PMDA with a series of methylbenzenes by TDDFT  
**Amit S. Tiwary**, *J. Indian Chem. Soc.*, **96** (2019) 659-665. Impact Factor-0.233, Citations-01

## Papers Presented in Seminars/Conferences

Sl. No.	Title of Lecture delivered / Paper presented / Paper published in conference	Title of Conference / Seminar etc., Date	Organized by	International (abroad/with in Country)/ National/
1	Ground State Geometry and Charge Transfer Transition Energy of the Toluene-ICl Molecular Complex: An <i>Ab Initio</i> and TDDFT Study	Advanced Spectroscopy, Theoretical Chemistry, Synthesis, Reactivity and Structure Evaluation <b>25-27<sup>th</sup> April 2008</b>	Department of Chemistry, The University of Burdwan	National
2	Mechanism of deamination of primary aliphatic amines: A DFT/TST study	Advanced Spectroscopy, Theoretical Chemistry, Synthesis, Reactivity and Structure Evaluation <b>20-22<sup>nd</sup> February, 2009</b>	Department of Chemistry, The University of Burdwan	National
3	Ab initio and TDDFT study of some buckybowls	Recent trends in Chemistry <b>25-26<sup>th</sup> February, 2010</b>	Department of Chemistry, Bidhan Chandra College, Asansol	National
4	Large Hadron Collider: To understand what world is made of	History of Physics <b>6-7<sup>th</sup> January, 2012</b>	Department of Physics, Netaji Mahavidyalaya, Arambagh, Hooghly	National
5	Mechanism of deamination of cytosine by Nitrous Acid: Ab initio DFT/TST study	"Frontier in Chemistry" <b>4-5<sup>th</sup> Dec, 2013</b>	Dept. of Chem., MUC Women's College	National
6	Theoretical Modelling: A green compliment to experiments- Deamination of Cytosine to Uracil as a test case	"The Biggest Challenge of Green Chemistry" <b>8-9<sup>th</sup> Oct, 2015</b>	Dept. of Chem AKPC Mahavidyalaya, Bengai, Hooghly	National

## Important Seminars/Conferences Attended

- **Celebration of Chemistry**, August 03, 2004 organized by The University of Burdwan in assistance with Chemical Research Society in India
- U.G.C. sponsored National Level Two-Day Seminar on “**New Vistas of Energy Search, Problems and Prospects**”, March 31 & April 01, 2007 organized by Netaji Mahavidyalaya, Arambagh, Hooghly.
- U.G.C. sponsored National Level Three-Day Seminar on “**Advanced Spectroscopy, Theoretical Chemistry, Synthesis, Reactivity and Structure Evaluation**”, 25-27<sup>th</sup> April, 2008, organized by Department of Chemistry, The University of Burdwan, Burdwan – 713104.
- U.G.C. sponsored National Level Three-Day Seminar on “**Advanced Spectroscopy, Theoretical Chemistry, Synthesis, Reactivity and Structure Evaluation**”, 20-22<sup>nd</sup> February, 2009 organized by Department of Chemistry, The University of Burdwan, Burdwan – 713104.
- U.G.C. sponsored National Level Two Day Seminar on “**Application of Spectroscopy: Atomic to Molecular Systems**”, 20-21<sup>st</sup> March, 2009 organized by PG Department of Chemistry, Vivekananda Mahavidyalaya, Burdwan,
- U.G.C. sponsored National Level Two Day Seminar on “**Recent trends in Chemistry**”, 25-26<sup>th</sup> Feb, 2010 organized by Department of Chemistry, Bidhan Chandra College, Asansol,
- U.G.C. sponsored National Level Two Day Seminar on “**Chemistry: A pathway to Biological processes**”, 24-25<sup>th</sup> Sept, 2010 organized by Department of Chemistry, Hooghly Mohasin College,
- U.G.C. sponsored National Level Three Day Seminar on “**International year of Chemistry: Chemistry in our lives under the thrust area: Design, Synthesis, Interaction, Chemical and Biochemical Activities of Different Functional Molecules**”, 15-17<sup>th</sup> March, 2011 organized by Department of Chemistry, The University of Burdwan.
- U.G.C. sponsored National Level Two Day Seminar on “**Recent Advances in Chemical Sciences and Related Areas**”, 18-19<sup>th</sup> Nov, 2011 organized by Department of Chemistry, S.G.B. College, Bagati
- U.G.C. sponsored National Level Two Day Seminar on ‘**History of Physics**’, 6-7<sup>th</sup> January, 2012 organized by the Department of Physics, Netaji Mahavidyalaya, Arambagh, Hooghly
- U.G.C. sponsored National Level Two Day Seminar on ‘**Recent Advances in E-Technology**’ 24-25<sup>th</sup> February, 2012 organized by the Department of Physics, Netaji Mahavidyalaya, Arambagh, Hooghly
- U.G.C. sponsored National Level Two Day Seminar on ‘**Conservation of Blue Carbon Sink: An approach towards safe environment**’, 11-12<sup>th</sup> April, 2012 organized by the Department of Physics, Netaji Mahavidyalaya, Arambagh, Hooghly

- U.G.C. sponsored National Level Two Day Seminar on ‘**Conservation of Blue Carbon Sink: An approach towards safe environment**’, 25-26<sup>th</sup> September, 2013 organized by the Department of Physics, Netaji Mahavidyalaya, Arambagh, Hooghly
- U.G.C. sponsored National Level Two Day Seminar on ‘**Quality Assurance Initiatives in Higher Education: Challenges, Trends and Priorities**’, 25-26<sup>th</sup> September, 2012 organized by MUC Women’s College, Burdwan
- U.G.C. sponsored National Level Two Day Seminar on ‘**Current Trend in Chemistry**’, 17-18<sup>th</sup> February 2014 organized by Vivekananda Mahavidyalaya, Burdwan
- U.G.C. sponsored National Level Three Day Seminar on ‘**Science Academies’ Lecture Workshop on “Frontiers in Chemistry: Fundamentals and Application**’, 6-8<sup>th</sup> December, 2017 organized by B.N. Mahavidyalaya, Itachuna, Hooghly
- National Level One Day Seminar on ‘**Current Trend in Chemistry**’, 5<sup>th</sup> February, 2018 organized by The Government College of Education, Burdwan

## Research Projects Completed

Successfully completed two Minor Research Projects under the financial assistance of UGC, New Delhi.

1. Following the path of reaction between primary amines and Nitrous acid by ab-initio and density Functional Theory (**Project Sanction Letter No: F.PSW-106/06-07(ERO) dated 10.02.2007**) during the period March 2007- Feb-2009.
2. Charge Transfer Interaction of Biomolecules: Theoretical Study using recent functional of DFT (**Project Sanction Letter No: F.PSW-038/15-16(ERO) dated 03.02.2017**) during the period March 2017- Feb-2019

## Awards and Honours Received

1. Qualified GATE (Graduate Aptitude Test in Engineering, 2000)
2. Qualified Lectureship-NET in the Joint CSIR-UGC National Eligibility Test (June, 2000)
3. Qualified Lectureship-NET in the Joint CSIR-UGC National Eligibility Test (July, 2001)
4. Qualified JRF-NET in the Joint CSIR-UGC National Eligibility Test (December, 2001)