

Dr Tanmoy Chakraborty

Journal Publications

1. Prabhat Ranjan, Shalini, **Tanmoy Chakraborty***(Accepted): A Review on Nanoalloy Clusters: Theory to Applications; *Recent Patents on Engineering*;
DOI: [10.2174/1872212114666200117111112](https://doi.org/10.2174/1872212114666200117111112)
2. Prabhat Ranjan, **Tanmoy Chakraborty***, Ajay Kumar (Accepted): Density Functional Study of Structures, Stabilities and Electronic Properties of AgAu_n^λ ($\lambda = 0, \pm 1; n=1-12$) Clusters: Comparison with Pure Gold Clusters, *Material Science - Poland*
3. Hiteshi Tandon, Prabhat Ranjan, **Tanmoy Chakraborty***, Vandana Suhag (2020): Polarizability: a promising descriptor to study chemical–biological interactions; *Molecular Diversity*, DOI: [10.1007/s11030-020-10062-w](https://doi.org/10.1007/s11030-020-10062-w)
4. Hiteshi Tandon, Prabhat Ranjan, **Tanmoy Chakraborty***, Vandana Suhag (2020): Computation of absolute radii of 103 elements of the periodic table in terms of nucleophilicity index; *Journal of Mathematical Chemistry*, Vol 58; DOI: [10.1007/s10910-020-01117-2](https://doi.org/10.1007/s10910-020-01117-2)
5. Prabhat Ranjan*, **Tanmoy Chakraborty*** (2020): Structure and Electronic Properties of Au_nPt ($n=1-8$) Nanoalloy Clusters: The Density Functional Theory Study; *Journal of Nanoparticle Research*, Vol 22; DOI: [10.1007/s11051-019-4745-5](https://doi.org/10.1007/s11051-019-4745-5)
6. Prabhat Ranjan, **Tanmoy Chakraborty*** (2020): A comparative study of structure, stabilities and electronic properties of neutral and cationic $[\text{AuSin}]^\lambda$ and $[\text{Sin}+1]^\lambda$ ($\lambda = 0, +1; n=1-12$) nanoalloy clusters; *Materials Today Communications*, Vol(22); DOI: [10.1016/j.mtcomm.2019.100832](https://doi.org/10.1016/j.mtcomm.2019.100832)
7. Jing Chang, Tanmoy Chakraborty, Raman Carbo-Dorca* (2020): Theoretical discussion on the double slit experiment and beyond: The Hückel (HMO) connection, *Trends in Physical Chemistry*, Vol 19
8. Shalini Choudhary, Prabhat Ranjan, **Tanmoy Chakraborty*** (2019): Atomic polarizability: A periodic descriptor; *Journal of Chemical Research*; DOI: [10.1177/1747519819889936](https://doi.org/10.1177/1747519819889936)
9. Prabhat Ranjan, Pancham Kumar, **Tanmoy Chakraborty***, Manisha Sharma, Sushella Sharma (2020): A study of structure and electronic properties of chalcopyrites semiconductor invoking Density Functional Theory; *Materials Chemistry and Physics*, Vol(241); DOI: [10.1016/j.matchemphys.2019.122346](https://doi.org/10.1016/j.matchemphys.2019.122346)
10. Ramon Carbó-Dorca*; **Tanmoy Chakraborty** (2019): Divagations about the periodic table: Boolean hypercube and quantum similarity connections, *Journal of*

11. Ramon Carbó-Dorca*; **Tanmoy Chakraborty (2019)**: Hypercubes defined on n-ary sets, the Erdős–Faber–Lovász conjecture on graph coloring, and the description spaces of polypeptides and RNA; *Journal of Mathematical Chemistry*, Vol(57); DOI: [10.1007/s10910-019-01065-6](https://doi.org/10.1007/s10910-019-01065-6)
12. Hiteshi Tandon, **Tanmoy Chakraborty***, Vandana Suhag (2019): A Model of Atomic Compressibility and Its Application in QSAR Domain for Toxicological Property Prediction; *Journal of Molecular Modeling*, Vol 25 (10); DOI: [10.1007/s00894-019-4199-9](https://doi.org/10.1007/s00894-019-4199-9)
13. Hiteshi Tandon, **Tanmoy Chakraborty***, Vandana Suhag (2019): A New Scale of Electrophilicity Index Invoking Force Concept; *Journal of Structural Chemistry*; DOI: [10.26902/JSC_id49735](https://doi.org/10.26902/JSC_id49735)
14. Hiteshi Tandon, **Tanmoy Chakraborty***, Vandana Suhag (2019): A New Scale of Atomic Static Dipole Polarizability, *Journal of Mathematical Chemistry*, Vol 57 (9); DOI: [10.1007/s10910-019-01055-8](https://doi.org/10.1007/s10910-019-01055-8)
15. Hiteshi Tandon, **Tanmoy Chakraborty***, Vandana Suhag (2019); A New Model of Atomic Nucleophilicity Index and Its Application in the Field of QSAR, *International Journal of Quantitative Structure-Property Relationships*, Vol 4 (99); DOI: [10.4018/IJQSPR.2019070104](https://doi.org/10.4018/IJQSPR.2019070104)
16. Hiteshi Tandon, **Tanmoy Chakraborty***, Vandana Suhag (2019): A Brief Review on Importance of DFT in Drug Design, *Research in Medical & Engineering Sciences*, Vol 7 (4). RMES.000668, DOI: [10.31031/RMES.2019.07.00068](https://doi.org/10.31031/RMES.2019.07.00068)
17. Prabhat Ranjan, **Tanmoy Chakraborty*** (2019): Density Functional Approach: To Study Copper Sulfide Nanoalloy Clusters; *Acta Chimica Slovenica (published by Slovenian Chemical Society)*, Vol 66; DOI: [10.17344/acsi.2018.4762](https://doi.org/10.17344/acsi.2018.4762)
18. Prabhat Ranjan, **Tanmoy Chakraborty*** (2018): A DFT Study of Vanadium Doped Gold Nanoalloy Clusters, *Key Engineering Materials*, Vol 777; DOI: [10.4028/www.scientific.net/KEM.777.183](https://doi.org/10.4028/www.scientific.net/KEM.777.183)
19. Shalini, Hiteshi Tandon, **Tanmoy Chakraborty*** (2017): Molecular Electrophilicity Index – A Promising Descriptor for Predicting Toxicological Property, *Journal of Bioequivalence and Bioavailability*, Vol 9 (6); DOI: [10.4172/jbb.1000356](https://doi.org/10.4172/jbb.1000356)
20. Prabhat Ranjan, **Tanmoy Chakraborty***, Ajay Kumar (2017): Computational Investigation of Cationic, Anionic and Neutral Ag₂AuN (N=1-7) Nanoalloy Clusters, *Physical Sciences Reviews*, Vol 2; DOI: [10.1515/psr-2016-0112](https://doi.org/10.1515/psr-2016-0112)
21. Prabhat Ranjan, **Tanmoy Chakraborty***, Ajay Kumar (2017): Computational Study of Au Doped Cu Nanoalloy Clusters, *Nano Hybrids and Composites*, Vol 17 (62);

- DOI: [10.4028/www.scientific.net/NHC.17.62](https://doi.org/10.4028/www.scientific.net/NHC.17.62)
22. Prabhat Ranjan, Seema Dhail, Srujana Venigalla, Ajay Kumar, Lalita Ledwani, **Tanmoy Chakraborty***(2015): A theoretical analysis of bi-metallic (Cu-Ag)_{n=1-7} nano alloy clusters invoking DFT based descriptors, *Materials Science - Poland*, Vol 33(4); DOI: [10.1515/msp-2015-0121](https://doi.org/10.1515/msp-2015-0121)
 23. Seema Dhail, **Tanmoy Chakraborty*** (2015): Theoretical Study of Lamivudine Derivatives Invoking DFT based Descriptors, *International Journal of Chemoinformatics and Chemical Engineering*, Vol 4 (2); DOI: [10.4018/IJCCE.2015070103](https://doi.org/10.4018/IJCCE.2015070103)
 24. Srujana Venigalla, Seema Dhail, Prabhat Ranjan, Shalini, **Tanmoy Chakraborty*** (2014): Computational Study about Cytotoxicity of Metal Oxide Nanoparticles Invoking Nano-QSAR Technique, *New Frontiers in Chemistry (Former: Ann. West Univ. Timisoara – Series Chem.)*, Vol 23 (2); DOI: [newfrontchem.iqstorm.ro/upload/12_NFC-23-2_Venigalla%20et%20al.pdf](https://doi.org/newfrontchem.iqstorm.ro/upload/12_NFC-23-2_Venigalla%20et%20al.pdf)
 25. Prabhat Ranjan, Srujana Venigalla, Ajay Kumar, **Tanmoy Chakraborty*** (2014): Theoretical study of Bi-metallic AgmAu_n; (m+n=2-8) Nano alloy clusters in terms of DFT Based Descriptors, *New Frontiers in Chemistry (Former: Ann. West Univ. Timisoara – Series Chem.)*, Vol 23 (2); DOI: [newfrontchem.iqstorm.ro/upload/11-NFC-23-2_Ranjan%20et%20al.pdf](https://doi.org/newfrontchem.iqstorm.ro/upload/11-NFC-23-2_Ranjan%20et%20al.pdf)
 26. Prabhat Ranjan, **Tanmoy Chakraborty***(2013): Quantum Mechanical Study of Some Atomic Properties, *Journal of International Academy of Physical Sciences*, Vol 17(3); DOI: www.iaps.org.in/journal/index.php/journaliaps/article/view/40>
 27. Sumanta Nayek, Suprakash Roy, Suvanka Dutta, Rajnarayan Saha*, and **Tanmoy Chakraborty** (2013): Dynamics of Metal Distribution in Cultivated Soil and Vegetables in Vicinity to Industrial Deposition: An Inference to Chemical Contamination of Food Chain, *International Journal of Chemoinformatics and Chemical Engineering*, Vol 3(2); DOI: [10.4018/ijcce.2013070109](https://doi.org/10.4018/ijcce.2013070109)
 28. **Tanmoy Chakraborty**, Dulal C. Ghosh* (2012): Correlation of the Drug Activities and Identification of the Reactive Sites in the Structure of Some Anti-Tuberculour Juglone derivatives in terms of the Molecular Orbital and the Density Functional Descriptors, *International Journal of Chemical Modeling*, Vol 4 (4)
 29. **Tanmoy Chakraborty**, Dulal C. Ghosh* (2011): Correlation of the Drug Activities of Some Anti-Tubercular Chalcone derivatives in Terms of the Quantum Mechanical Reactivity Descriptors, *International Journal of Chemoinformatics and Chemical Engineering*, Vol 1 (2), DOI: [10.4018/ijcce.2011070104](https://doi.org/10.4018/ijcce.2011070104)
 30. **Tanmoy Chakraborty**, Kamarujjaman Gazi and Dulal C. Ghosh* (2010): Computation of

the Atomic Radii through the Conjoint Action of the Effective Nuclear Charge and the Ionization Energy, *Molecular Physics*, Vol 108 (16); DOI: [10.1080/00268976.2010.505208](https://doi.org/10.1080/00268976.2010.505208)

31. **Tanmoy Chakraborty**, Dulal C. Ghosh* (2010); Computation of the Dipole Moment of Some Heteronuclear Diatomic Molecules in terms of Revised Electronegativity Scale of Allred and Rochow, *European Journal of Chemistry*, Vol 1 (3); DOI: [10.5155/eurjchem.1.3.182-188.72](https://doi.org/10.5155/eurjchem.1.3.182-188.72)
32. **Tanmoy Chakraborty**, Dulal C. Ghosh* (2010); Computation of the Inter Nuclear Distances of Some Hetero nuclear Diatomic Molecules in terms of the Revised Electronegativity Scale of Gordy, *The European Physical Journal D*, Vol 59 (2); DOI: [10.1140/epjd/e2010-00159-7](https://doi.org/10.1140/epjd/e2010-00159-7)
33. Dulal C. Ghosh*, **Tanmoy Chakraborty** (2009): Computation of the dipole moments of some heteronuclear diatomic molecules in terms of the revised electronegativity scale of Gordy, *Journal of Molecular Structure: Theochem (Presently continued as Computational and Theoretical Chemistry)*, Vol 916; DOI: [10.1016/j.theochem.2009.09.009](https://doi.org/10.1016/j.theochem.2009.09.009)
34. Dulal C. Ghosh*, **Tanmoy Chakraborty**, Bhabatosh Mandal (2009); The electronegativity scale of Allred and Rochow: revisited, *Theoretical Chemistry Accounts*, Vol 124; DOI: [10.1007/s00214-009-0610-4](https://doi.org/10.1007/s00214-009-0610-4)
35. Dulal C. Ghosh*, **Tanmoy Chakraborty** (2009): Gordy's Electrostatic Scale of Electronegativity Revisited, *Journal of Molecular Structure: Theochem (Presently continued as Computational and Theoretical Chemistry)*, Vol 906
DOI: [10.1016/j.theochem.2009.04.007](https://doi.org/10.1016/j.theochem.2009.04.007)
36. Dulal C Ghosh*, Raka Biswas, **Tanmoy Chakraborty**, Nazmul Islam and Sandip K. Rajak (2008): The Wave Mechanical Evaluation of the Absolute Radii of Atoms, *Journal of Molecular Structure: Theochem (Presently continued as Computational and Theoretical Chemistry)*, Vol 865; DOI: [10.1016/j.theochem.2008.06.020](https://doi.org/10.1016/j.theochem.2008.06.020)
37. Dulal C. Ghosh*, **Tanmoy Chakraborty**, Nazmul Islam, Raju Roy and Sanjib Kr.Mondal (2007): Quantum Mechanical Evaluation of Atomic Radii of 86 Elements of Periodic Table, *Chemistry in North Bengal University, Annual Journal*, Vol 1

Book Chapters/ Conference Proceedings

1. Hiteshi Tandon, Shalini, Prabhat Ranjan, Vandana Suhag, **Tanmoy Chakraborty** (2019): Book Chapter - A Review on Computational Study of Carbon Nanotubes, "Carbon Nanotubes and Nanoparticles: Current and Potential Applications" by *Apple Academic Press*; ISBN: 9780429463877
2. Edited book by **Tanmoy Chakraborty**, Ramon Carbo-Dorca (2018): "Theoretical and Quantum Chemistry at the Dawn of the 21st Century" 1st Edition, published by *Apple Academic Press, Taylor & Francis group*; ISBN 9781771886826 - CAT# K345241

3. Suprakash Roy, Seema Dhail, Subhendu Naskar and **Tanmoy Chakraborty** (2013): Correlation of the Experimental and Theoretical Study for the Cyclisation Reaction of Mesoionic Heterocycle Imidazo[1,5-a]pyridines in terms of the Density Functional Descriptors, Published in edited research book – “Computational and Experimental Chemistry- Developments and Applications”, Published by *Apple Academic Press and Distributed by Taylor & Francis Group*; ISBN-13: 978-1926895291
4. Prabhat Ranjan, Ajay Kumar and **Tanmoy Chakraborty** (2014): Computational study of Nano-materials Invoking DFT based descriptors, Published in Environmental Sustainability: “Concepts, Principles, Evidences and Innovations” (Edited Research Book), Published by *Excellent Publishing House, New delhi*; ISBN: 978-93-83083-75-6
5. Seema Dhail, Lalita Ledwani and **Tanmoy Chakraborty** (2016): A survey of QSAR- Approach to Drug Design, Published in edited research book – “Research Methodology in Chemical Sciences: Experimental and Theoretical Approach”, by *Apple Academic Press and Distributed by Taylor & Francis Group*; ISBN: 9781315366616
6. Prabhat Ranjan, Srujana Venigalla, Ajay Kumar and **Tanmoy Chakraborty** (2016): A Theoretical Analysis of Bi-metallic Ag-Au; $(n=1-7)$ Nano Alloy Clusters Invoking DFT based Descriptors, Published in edited research book – “Research Methodology in Chemical Sciences: Experimental and Theoretical Approach”, by *Apple Academic Press and Distributed by Taylor & Francis Group*; ISBN: 9781315366616
7. Prabhat Ranjan, Ajay Kumar and **Tanmoy Chakraborty**: Name of Conference Proceedings (IEEE): International Conference on Futuristic Challenge in Computational Science and Knowledge Management; Name of Book Chapter: Computational Study of CuAg ($n=1-8$) Nano alloy Clusters Invoking DFT Based Descriptors;; (ISBN no. 978-1-4799-8432-9).

Conferences

- Keynote Presentation – June 2019
Global Scientific Event on Atomic, Molecular, and Optical
Physics (GSEAMO)-2019 – Dubai, UAE
- Invited lecture – May 2018
2018 International Conference on Computational Chemistry and
Toxicology in Environmental Science (2018 CCTES)
National Chung Hsing University - Taiwan
- Keynote Presentation – October 2015
4th International Summit on GMP, GCP Quality, Hyderabad –
India
- Invited lecture – August 2014
Virtual Conference on Computational Chemistry –
University of Mauritius – Mauritius
- Paper Presentation – June 2014
16th International Workshop on Quantitative Structure-Activity
Relationships in Environmental and Health Sciences (QSAR2014)
- Milan, Italy
- Paper Presentation – May 2014
2nd Rajasthan Science Congress -
Dr. K.N.Modi University – Rajasthan, India
- Paper Presentation – April 2014
Manipal Research Colloquium –
Manipal Academy of Higher Education - Manipal,
India
- Paper Presentation at Agriculture, Food Engineering and March 2014
Environmental Sciences- Sustainable Approaches”
(AFEESSA- 2014) - Jawaharlal Nehru University,
India
- Paper presentation – October 2012
International Conference ‘IWCEM-2012’
National University of Singapore
- Poster presentation – February 2009
11th CRSI NATIONAL SYMPOSIUM IN CHEMISTRY –
National Chemical Laboratory - India.
- Poster Presentation – December 2009
International Symposium ‘Of Molecules and Materials (OMAM)’
–

IISER - India

Paper presentation –
National Seminar on Current Trends in Chemistry-I (NSCTC-I) –
University of Kalyani, India.

January 2008

Participated
National Workshop on application of Bio informatics in Molecular
Modeling, Data Analysis and System Biology –
University of Kalyani, India

March 2007

Poster presentation -
National Symposium on ‘Advances in Chemistry and
Environmental Impact’ –
North-eastern Hill University, Shillong, India

November 2006