

## Dr. Purav M. Badani

Designation : Assistant Professor in Chemistry  
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### Academic Record

Degree	University	Year of Passing	Class
B.Sc. (Chemistry)	University of Mumbai	2007	Distinction
M.Sc. (Physical Chemistry)	University of Mumbai	2009	Distinction <b>(University Gold Medalist)</b>
Maharashtra SET (Chemical Sciences)	-----	2011	-----
PhD (Chemistry)	B.A.R.C., University Of Mumbai	2015	-----

### Positions held

Assistant Professor	Wilson College, Chowpatty, Mumbai: 400007	Oct, 2013 – Mar, 2014
Assistant Professor	Department of Chemistry, University of Mumbai	Mar, 2014 – till date

### Membership of professional bodies

1. Life member of Society for Materials Chemistry (LM - 314).
2. Life member of Indian Society for Mass Spectrometry (LM - 750)
3. Life member of Indian Society for Radiation and Photochemical Sciences.
4. Life member of Indian Science Congress Association

## Awards and Honors

2009	Prof. A. N. Kothare Gold Medal, University of Mumbai
2009	Dr. B. N. Desai Gold Medal, University of Mumbai
2009	Dr. K. A. Hamied's Chemistry Prize, University of Mumbai
2009 - 2011	Junior Research Fellowship, Department of Atomic Energy, Government of India
2011 - 2013	Senior Research Fellowship, Department of Atomic Energy, Government of India

## Topics taught

At M.Sc. (Part 1): Quantum Chemistry

At M.Sc. (Part 2): Solid State Chem., Photo-Chemistry & Advance Instrumental Techniques.

## Research Interest

- *Computational Chemistry*: Molecular Modeling and reaction dynamics
- *Experimental Chemistry*: Synthesis of nanoparticles and its application in degradation of dyes

## Research Highlights

a) Past:

Previously, I was involved in performing research work related to laser-cluster interaction in gas-phase. In context of laser-cluster interaction, clusters efficiently couple with the laser radiation thereby extracting huge amount of energy from the optical field. This results in extensive stripping of electrons from the cluster constituents which leads to buildup of excessive positive charge on cluster. The cohesive energy tries to hold the clusters while the electrostatic repulsion, arising from positive charges, forces the cluster to expand. At a stage when the repulsive Coulombic energy of cluster overcomes the total cohesive energy, cluster disintegrates violently. This is manifested in terms of generation of multiply charged atomic ions with huge kinetic energies, which is referred as Coulomb Explosion.

The aim and objectives of our investigations were as follows.

- To explore the change in photo-ionization behavior of molecules as they aggregate to form clusters.
- To identify the factors influencing the efficiency of laser-cluster interaction.

- c. To investigate the variation in photo-ionization behavior of pure and doped atomic/molecular clusters.
- d. To understand the mechanism by which clusters exhibit multiple ionization and subsequent Coulomb explosion phenomena under gigawatt intensity laser field.

*(Above research work was carried out at Chemistry Division, B.A.R.C., Mumbai under the supervision of Dr. R. K. Vatsa)*

b) Current:

Presently our group (at Computational and Theoretical Science Laboratory, University of Mumbai) is involved in performing electronic structure calculations on series of atmospherically important species. For instance, halocarbons, that are released in the atmosphere both from natural as well as man-made sources, has a pronounce effect on environment. On interacting with UV, vacuum ultraviolet (VUV) and other ionizing radiations of solar and cosmic origin, they generate reactive halogen species. These halogen species contribute considerably to the loss of stratospheric ozone which is vital to life. Hence, the research work is directed to explore the dissociation/ionization dynamics of uni- i.e.  $C_nH_{2n+1}X$  and multi-halogenated alkyls i.e.  $C_nH_{2n}X_2$  and  $C_nH_{2n}XY$  (where X, Y = F, Cl, Br, etc.), which are under the influence of ionizing radiations. The objectives of the work is a follows:

- Exploring the dissociation/ionization dynamics of uni- i.e.  $C_nH_{2n+1}X$  and multi-halogenated alkyls i.e.  $C_nH_{2n}X_2$  and  $C_nH_{2n}XY$  (where X, Y = F, Cl, Br, etc.), which are under the influence of ionizing radiations.
- Exploiting the reaction pathways responsible for generation of reactive halogen species such as X,  $X^+$ ,  $X_2$ ,  $X_2^+$ , XY,  $XY^+$ , etc.
- Identifying the effect of substitution on reaction dynamics of halocarbons.
- Investigating the mechanism of  $X_2$ ,  $X_2^+$ , XY and  $XY^+$  elimination from multi-halogenated alkyls.

Thus, our research work primarily focused to identify the mechanism of dehalogenation processes which will act as sink in removal of these compounds from the biosphere.

*(Above research work is supported by SERB-DST, Government of India. through Young Scientist Scheme No. YSS/2015/001106)*

## Research Project

Sr. No	Title	Funding agency	Amount (in Rs.)	Status
1	Exploring the dissociation/ionization dynamics of molecules through electronic structure calculations (YSS/2015/001106)	DST-SERB	29.01 lakhs	ongoing

## Journal Papers

- 1 T. Twade, S. Wagh, J. V. Sapre, V. N. Khose, **P. M. Badani**, A. V. Karnik  
“Chiral Base-catalyzed Asymmetric Diels-Alder Reaction: Achiral Flexible Heterocyclic Arm Induced Unusual Reversal of Enantioselectivity”  
*Tetrahedron: Asymmetry* (Accepted).
- 2 **P. M. Badani**, S. Das, P. Sharma and R. K. Vatsa.  
“Mass spectrometric and charge density studies of organometallic clusters photoionized by gigawatt laser pulses”  
*Mass Spectrometry Review* DOI: 10.1002/mas.21469. (Impact factor 8.053)
- 3 S. Das, P. Sharma, **P. M. Badani** and R. K. Vatsa.  
“Ionization of methyl iodide clusters using nanosecond laser pulses: detection of multiply charged positive ions, negative ions and energetic electrons”  
*RSC Advances* 5 (2015) 8887. (Impact factor 3.708)
- 4 **P. M. Badani**, S. Das, P. Sharma and R. K. Vatsa.  
“Generation of multiply charged tin and carbon ions in low intensity Coulomb explosion of tetramethyl tin clusters: Role of screening effects”  
*International Journal of Mass Spectrometry* 358 (2014) 36. (Impact factor 2.227)
- 5 **P. M. Badani**, S. Das, P. Sharma, KRS Chandrakumar and R. K. Vatsa.  
“Evidence for charge-induced dipole reaction in laser ionized van der Waals clusters: A case of Fe<sup>2+</sup> reacting with argon atoms inside a cluster.”  
*RSC Advances* 4 (2014) 2339. (Impact factor 3.708)
- 6 S. Das, **P. M. Badani**, P. Sharma and R. K. Vatsa.  
“Diverse photochemical behavior of dibromodifluoromethane (CF<sub>2</sub>Br<sub>2</sub>) monomer and cluster under gigawatt intensity laser fields.”  
*RSC Advances* 3 (2013) 12867. (Impact factor 3.708)
- 7 **P. M. Badani**, S. Das, P. Sharma & R. K. Vatsa.  
“Photoionization of atomic and molecular clusters doped with low ionization energy molecules: Effect of laser wavelength, intensity and cluster composition.”  
*International Journal of Mass Spectrometry* 348 (2013) 53. (Impact factor 2.227)

- 8 A. Y. Desai, **P. M. Badani**, S. Roy, A. D. Sawant.  
“Application of topology in calculation of Bond Order.”  
*International Journal of Chemistry* 1 (2012) 38.
- 9 S. Das, **P. M. Badani**, P. Sharma and R. K. Vatsa.  
“Interaction of xenon clusters with nanosecond laser pulses: A size-dependent study.”  
*Chemical Physics Letters* 552 (2012) 13. (Impact factor 2.088)
- 10 **P. M. Badani**, S. Das, P. Sharma and R. K. Vatsa.  
“Effect of cluster expansion on photo-ionization behavior of iron pentacarbonyl doped inert gas cluster.”  
*Rapid Communication in Mass Spectrometry* 26 (2012) 2204. (Impact factor 2.642)  
(P.T.O.)
- 11 P. Sharma, S. Das, **P. M. Badani** and R. K. Vatsa.  
“Photochemistry of  $(\text{CH}_3\text{SCH}_3)_n$  and  $(\text{CH}_3\text{SSCH}_3)_n$  clusters at 355 and 532 nm using time-of-flight mass spectrometer.”  
*Indian Journal of Physics* 86 (2012) 195. (Impact factor 1.785)
- 12 S. Das, **P. M. Badani**, P. Sharma and R. K. Vatsa.  
“Coulomb explosion phenomenon using gigawatt intensity laser fields: an exotic realm of laser-cluster interaction.”  
*Current Science* 100 (2011) 1008. (Impact factor 0.833)
- 13 S. Das, **P. M. Badani**, P. Sharma, R. K. Vatsa, D. Das, A. Majumder and A. K. Das.  
“Multiphoton ionization and Coulomb explosion of  $\text{C}_2\text{H}_5\text{Br}$  clusters: a mass spectrometric and charge density study.”  
*Rapid Communication in Mass Spectrometry* 25 (2011) 1028. (Impact factor 2.642)
- 14 **P. M. Badani**, S. Das, M. V. Rao, P. Sharma and R. K. Vatsa.  
“Interaction of nanosecond laser pulse with tetramethyl silane  $(\text{Si}(\text{CH}_3)_4)$  clusters: Generation of multiply charged silicon and carbon ions.”  
*AIP Advances* 1 (2011) 042164. (Impact factor 1.591)

### Poster presentations at various symposia/conferences

1. “Photochemistry of tetramethyl silane clusters.”, **P. M. Badani**, S. Das, P. Sharma and R. K. Vatsa. Presented at Trombay Symposium in Radiation and Photochemistry, 2010.
2. “Clusters as Versatile Source for Generation of Multiply Charged Ions.”, **P. M. Badani**, Venkateswara Rao, S. Das, P. Sharma and R. K. Vatsa. Presented at International Symposium in Materials Chemistry, 2010.
3. “Photo-ionization behavior of Tetramethyl silane doped inert-gas clusters.”, **P. M. Badani**, S. Das, M. V. Rao, P. Sharma and R. K. Vatsa. Presented at Trombay Symposium of Radiation & Photochemistry, 2012.
4. “Photo-ionization of Pure and Doped inert gas clusters”, **P. M. Badani**, S. Das, P. Sharma and R.K. Vatsa. Presented at Interdisciplinary Symposium in Materials Chemistry, 2012.

5. "Interaction of Fe(CO)<sub>5</sub> doped inert gas clusters with gigawatt intensity laser pulses." **P. M. Badani**, S. Das, P. Sharma and R.K. Vatsa. Presented at Meeting on Spectroscopy and Dynamics of Molecules and Clusters, 2013.
6. "Photoionization of Fe(CO)<sub>5</sub> doped Xenon/SF<sub>6</sub> clusters using gigawatt intensity laser pulses.", **P. M. Badani**, S. Das, P. Sharma and R.K. Vatsa. Presented at 12<sup>th</sup> ISMAS-TRICON, 2013.
7. "Study of ionization processes in molecular clusters using mass spectrometry." **P. M. Badani** and R. K. Vatsa. Oral Presentation at 25<sup>th</sup> Research Scholars' Meet, 2013.
8. "Evidence of charge-induced dipole reaction in laser ionized van der Waals clusters: An experimental and theoretical investigation.", **P. M. Badani**, S. Das, KRS Chandrakumar, P. Sharma and R.K. Vatsa. Presented at Current Trends in Theoretical Chemistry, 2013.
9. "Catalytic degradation of methylene blue dye using silver nanoparticles." C. Pal and **P. M. Badani**. Presented at Advances and Innovations in Chemical Sciences, 2015.

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