

# Curriculum Vitae

## Subhasish Saha

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### Objective

To be associated with a progressive organization that provides an opportunity to apply my knowledge and skills in order to keep abreast with latest science trends and technologies.

### EDUCATIONAL QUALIFICATION

Qualification	School/Institute(Board/University)	Year of Passing	Marks(%)
Post-Doctoral Researcher	IISER Kolkata	2023- Continue	
Post-Doctoral Researcher	The Ohio State University, USA	2021- 2022	
P.hD	Indian Institute of Technology Patna	2016-2021	7.71 (CGPA)
B. Ed.	Kurukshetra University	2014-2015	54.00
M.Sc (PHYSICS)	Ramkrishna Mission Residential College,Narendrapur (University of Calcutta)	2014	70.80
B.Sc (PHYSICS HONS)	Dum Dum Motijheel College (West Bengal State University)	2012	60.13
XII	Naraindass Bangur Memorial Multipurpose High School(West Bengal Council Of Higher Secondary Education)	2008	77.00
X	Dum Dum Krishna Kumar Hindu Academy (West Bengal Board Of Secondary Education)	2006	69.50

Qualified All India Exam: GATE (2015) and NET (2015)

**Research Field: Computational Atomic and Molecular Physics**

- Photoionization dynamics of free and confined atom
- Electronic structure properties of confined atomic system

### Publications:

1. Photoionization dynamics of endohedrally confined atomic H and Ar: a contrasting study between compact versus diffused model potential, **S Saha**, A Thuppilakkadan, H R Varma and J Jose, *J. Phys. B: At. Mol. Opt. Phys.* 52 145001 (2019). <https://iopscience.iop.org/article/10.1088/1361-6455/ab1f16>

2. Shannon entropy as a predictor of avoided crossing in confined atoms, **S Saha** and J Jose, *Int J Quantum Chem.* 120 e26374 (2020). <https://doi.org/10.1002/qua.26374>
3. Photoionization phase shift and Wigner time delay of endohedrally confined atoms using transient phase methods, **S Saha**, A Thuppilakkadan, H R. Varma, J Jose, *Eur. Phys. J. Plus* 135:753 (2020). <https://doi.org/10.1140/epjp/s13360-020-00762-5>
4. Entropic uncertainty as a predictor of avoided crossing for confined system, **S Saha**, J Jose and P C Deshmukh, *Journal of Physics: Conference Series* 1412 122029 (2020). <https://doi.org/10.1088/1742-6596/1412/12/122029>
5. Shannon entropy as an indicator of correlation and relativistic effects in confined atoms, **S Saha** and Jobin Jose, *Physical. Rev. A.* 102, 052824 (2020). <https://doi.org/10.1103/PhysRevA.102.052824>
6. Sensitivity of correlation effects and Shannon entropy in Be@C<sub>60</sub> to the nature of confinement potentials, **S Saha** and Jobin Jose, *Phys. Scr.* 96 094012 (2021). <https://doi.org/10.1088/1402-4896/ac098c>
7. Impact of Charge Migration and the Angle-Resolved Photoionization Time Delays of the Free and Confined Atom X@C<sub>60</sub>, **S Saha**, S Banerjee, and J Jose, *Atoms* 2022, 10, 44. <https://doi.org/10.3390/atoms10020044>
8. Unusual behavior of Cooper minima of *ns* subshells in high-Z atoms, S Baral, **S Saha**, Km. A Dubey, J Jose, P C Deshmukh, A K Razavi and S T Manson, *Physical. Rev. A.* 105, 062819 (2022). <https://journals.aps.org/pr/abstract/10.1103/PhysRevA.105.062819>
9. Study of electron impact elastic scattering from Kr@C<sub>60</sub> and Xe@C<sub>60</sub> using a fully relativistic approach, D Mahato, L Sharma, S Baral, S Saha, J Jose, and R Srivastava, *J. Phys. B: At. Mol. Opt. Phys.* 55 165201 (2022). <https://iopscience.iop.org/article/10.1088/1361-6455/ac7b59>
10. Dramatic Relativistic Effects on the *ns* Dipole Angular Distribution Asymmetry Parameter,  $\beta_{ns}$ , of Heavy and Superheavy Elements. S. Baral , S. Saha , Km. A. Dubey , J. Jose 1 , P. C. Deshmukh, A. K. Razavi and S. T. Manson, *J. Phys. B: At. Mol. Opt. Phys.* 56 055003 (2023). <https://doi.org/10.1088/1361-6455/acb873>

### Conferences attended:

- (A) 7<sup>th</sup> Topical Conference of the Indian Society of Atomic and Molecular Physics (ISAMP), IISER and IIT Tirupati, January 6-8, 2018.
- (B) 13<sup>th</sup> Asian International Seminar on Atomic and Molecular Physics, TIFR and IIT Bombay, December 3-8, 2018.
- (C) 31<sup>st</sup> International Conference on Photonic, Electronic and Atomic Collisions (ICPEAC XXXI) in Caen and Deauville, France, July, 23-30, 2019.
- (D) International Conference on Quantum and Atom Optics, IIT Patna, December 16-18, 2018.
- (E) National Conference on Atomic, Molecular and Nano Sciences (NCAMNS-2019) in Aliah University, Kolkata, India, April 3-4, 2019.

## **Referees**

### **Dr. P. C. Deshmukh**

Mentor and Convener, Center for Atomic, Molecular, and Optical Sciences and Technologies  
(Joint Initiative of IIT Tirupati and IISER Tirupati)

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### **Dr. Hari Varma**

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### **Dr. Sangita Sen**

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## **Co-Curricular & Extra-Curricular Activities**

Hobbies include listening music, playing and watching Cricket, Movies etc.

## **Personal Profile**

Father's Name : JaharLal Saha  
Mother's Name : Provati Saha  
Nationality : Indian  
Sex : Male  
Category : General  
Marital status : Widower

## **Declaration**

I hereby declare that the above-mentioned information is correct up to my knowledge and I bear the responsibility for the correctness of the above-mentioned particulars.

**Place:** Kolkata  
**Date:** 23.07.2023

*Subhasish Saha*

# Research Summary

(1) **Photoionization dynamics** (cross section, angular asymmetry parameter, phase shift and Wigner time delay) of free and endohedrally confined atom ( $A@C_{60}$ ) are studied using single active electron approximation (SAE) and also relativistic many body techniques like relativistic random phase approximation (RRPA).

- In SAE approach, the phase shift and the corresponding attosecond time delay is determined by referring finite difference method (FD method) and the transient phase methods. Two transient phase methodologies are employed (A) comparing logarithmic derivatives of the analytical solution at shell boundaries and (B) Born approximation.
- In the RRPA approach (based on Time dependent Dirac-Fock theory), the charge migration (hybridization of atomic state and well state) is occurred at certain well depth of confinement. Impact of charge migration on the individual channel time delay and spin averaged angle dependent time delay are observed. Because of the anisotropy of the photoionization process the angle dependent time delay is important. The spherical spinor in the expression of transition amplitude contains the angle information in spherical harmonics. The interference between two different quantum paths, which lead to two different final state continua of different symmetry from the same initial bound state, makes the time delay angle sensitive.

(2) **Electronic structure properties** (energy spectrum, electron density distribution, avoided crossing phenomena, correlation and relativistic effects on Shannon entropy) of free and confined atom are studied using multi-configuration Dirac-Fock (MCDF) theory.

- Energy states reordering results from the energy level repulsion; those with the same symmetry do not cross each other. Rather they come close, and then they repel each other, exhibiting avoided crossing. As a consequence of this, mirroring the behaviour of the states also occurs, which is known as mirror collapse. The mirror collapse manifests as the exchange of information between the two states involved in avoided crossing. The existence of avoided crossings between the pairing states in the presence of the confinement environment manifests in Shannon entropy. The behavior of Shannon entropy shows that the states involved in this avoided crossing exchange their informational character due to mirror collapse.
- The influence of relativistic and correlation effects on the Shannon entropy of confined atoms have been investigated using MCDF theory. The correlation energy in  $Be@C_{60}$  is studied as a function of the depth of the confining potential to give some idea as to how *Shannon's correlation entropy* is sensitive to the minimum location of correlation energy. To see the prominent relativistic effects in the confined atom, *Shannon's relativistic entropy* of the valence subshell of  $Ba@C_{60}$  is scrutinized for different confinement parameters.

(3) Many spherically averaged static model potentials are introduced to realistically mimic the endohedral environment ( $C_{60}$ ) for a less complex calculation. In my thesis, Gaussian annular square well (GASW) model potential is proposed, which includes an average effect of 240 valence shell electrons and protons of the  $C_{60}$  cage. The contrast between the diffusive Gaussian annular square well (GASW) and the compact annular square well (ASW) model potential on the photoionization dynamics and electronic structure calculation are explored.

## Future Scope

[1] In my thesis, I have reported the electronic structure and dynamic properties of close shell atoms. There is scope to study these properties of open-shell atoms for the free and confined system.

[2] The correlation effects on Be@C<sub>60</sub> were portrayed only for two configurations (C<sub>1</sub>): $1s^2 (2s^2 + 2p_{1/2}^2 + 2p_{3/2}^2)$ , J=0, and (C<sub>2</sub>): $1s^2 (2s^2 + 2p_{1/2}^2 + 2p_{3/2}^2 + 3s^2)$ , J=0. There is a scope to enhance the terms in the CI expansion to see the alterations in the localization properties. Furthermore, other confined systems can be explored.

[3] The effect of charge migration on the angle-dependent time delay would be of interest for other atoms.

[5] A charged fullerene cage to confine an atom would cause Coulomb Confinement Resonances (CCR) in addition to the ordinary confinement resonances. Angle-dependent time delay studies of CCR can be performed in the future.

[6] High-harmonic generation (HHG) from the A@C<sub>60</sub> has not been studied in detail; hence such studies demand attention in the immediate future.

[7] Development of global potential energy surfaces of small molecular systems, quantum mechanical calculations of molecular spectroscopy, dynamics of photodissociation, and quantum reactive scattering.