



## Dr. Shubhadip Chakraborty

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*Department of Chemistry*

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## OVERVIEW

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I am an astrochemist. I work in the domain of spectroscopy of large carbonaceous molecules and apply my knowledge of spectroscopy for a deeper understanding of the chemistry of the interstellar medium. Very recently, I have started my independent career as an assistant professor in the Department of Chemistry, GITAM university, Bengaluru, India.

## RESEARCH INTERESTS

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- Identification of the carriers of the diffuse interstellar bands (DIBs) based on experimental and theoretical infrared spectroscopy of fullerenes.
- Far infrared spectroscopy of polycyclic aromatic hydrocarbons (PAHs) from an experimental and theoretical approach.
- Processing of interstellar dust analogues (silicates, polycyclic aromatic hydrocarbons, hydrogenated amorphous carbon etc.) using shock waves and their real time spectroscopy.
- Infrared spectroscopy of hot cosmic polycyclic aromatic hydrocarbons (PAHs) and Fullerenes for modeling the observed mid-infrared (MIR) emission profiles in various astronomical objects.
- Simulation of variable temperature anharmonic infrared spectra of PAHs using quantum chemical and molecular dynamics simulations.

## APPOINTMENTS

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### Assistant professor

06/09/2022-till now

*Department of Chemistry, GITAM university, Bengaluru, India*

### Postdoctoral researcher

02/05/2019-31/07/2022

*Institut de Physique de Rennes, UMR CNRS 6251 Université de Rennes1 Campus de Beaulieu 35042 Rennes Cedex, France*

### Postdoctoral Researcher

02/11/2016-30/11/2018

*Institut de Recherche en Astrophysique et Planetologie, Université de Toulouse, CNRS, CNES, 9 Av. du Colonel Roche, 31028 Toulouse Cedx 4, France*

### Postdoctoral Researcher

02/08/2015-30/09/2016

*Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore, India*

## EDUCATION

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### PhD Physical Chemistry (Spectroscopy)

03/07/2009-12/03/2016

Indian Institute of Science, Bangalore, India

**Thesis title:** Gas Phase Infrared Spectroscopy of Large Aromatic Molecules: Fermi Resonance in the C-H Stretching Region

#### Thesis advisor

Prof. Puspendu K. Das, Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore, India

### M.Sc. Chemistry with Physical Chemistry specialization

2007-2009

Indian Institute Engineering Science and Technology, Shibpur, Kolkata, India

**Thesis title:** Theoretical Investigation of Electronic Structure of Ketene at *ab-initio* limit

#### Thesis advisor

Prof. Sudip K. Chattopadhyay, Department of Chemistry, Indian Institute Engineering Science and Technology, Shibpur, Kolkata, India

### B.Sc. Honours in Chemistry

2003-2006

Bhairab Ganguly College, University of Calcutta, Kolkata, India

Chemistry) of the Indian Institute of Science, Bangaluru, India.

## PEER-REVIEWED JOURNAL PAPERS [\[statistics\]](#)

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19. A.Sivakumara, S. Sahaya Jude Dhas, P.Sivaprakash, A. DhayalRaj Raju SureshKumar, S.Arumugam, S.Prabhu, R.Ramesh, **S. Chakraborty**, S.A. Martin Britto Dhas, “[Shock wave recovery experiments on  \$\alpha\$ -V<sub>2</sub>O<sub>5</sub> nano-crystalline materials: A potential material for energy storage applications](#)”, *J. Alloys and Comps.* **929**, 17180 (2022).
18. A. Sivakumar, A. Rita, S. S. Jude. Dhas, K.P. J. Reddy, R. S. Kumar, A. Almansour, **S. Chakraborty**, K. Moovendaran, S. Jayavel, S. A. Martin Britto Dhas, “[Dynamic Shock Wave Driven Simultaneous Crystallographic and Molecular Switching between  \$\alpha\$ -Fe<sub>2</sub>O<sub>3</sub> and Fe<sub>3</sub>O<sub>4</sub> nanoparticles- A new finding](#)”, *Dalton Trans.* **51**, 9159 (2022).
17. A. Sivakumar, S. S. Jude Dhas, J. Tirupathy, K. P. J. Reddy, R. S. Kumar, A. Almansour, **S. Chakraborty**, S. A. Martin Britto Dhas , “[Switchable crystal–amorphous states of NiSO<sub>4</sub>·6H<sub>2</sub>O induced by a Reddy tube](#)”, *New. J. Chem.* **46**, 5091 (2022).
16. A. Sivakumar, S. Jude Dhas, **S. Chakraborty**, R. S. Kumar, A. Almansour, N. Arumugam, S.A. Martin Britto Dhas , “[Dynamic Shock Wave Induced Amorphous to Crystalline Switchable Phase Transition of Lithium Sulfate](#)”, *J. Phys. Chem. C* **126**, 3194 (2022).
15. O. Berne et al. , “[PDRs4All: A JWST Early Release Science Program on radiative feedback from massive stars](#)”, *Pub. Astro. Soc. Pacific.* **134**, 054301 (2022 ).
14. A. Sivakumar, P. Shailaja, M. Nandhini, S. Sahaya Jude Dhas, R. S. Kumar, A. I. Almansour, N. Arumugam, **S. Chakraborty** and S.A. Martin Britto Dhas, “[Ternary switchable phase transition of CaCO<sub>3</sub> by shock waves](#)”, *Ceramics International* **48**, 8457 (2021).

13. A. Sivakumar, P. Shailaja, S. S. J. Dhas, P. Sivaprakash, A. Almansour, R. S. Kumar, Suresh; N. Arumugam, A. Sonachalam, **S. Chakraborty**, S. A. Martin Britto Dhas, “[Dynamic Shock Waves Induced Switchable Phase Transition of Magnesium Sulfate Heptahydrate](#)”, *Crys. Growth Des.* **21**, 5050 (2021).
12. A. Sivakumar, V. Mowlika, S. S. J. Dhas, A. I. Almansour, R. S. Kumar, A. Natarajan, R. Robert, **S. Chakraborty** and S. A. Martin Britto Dhas, “[Assessment of shock resistance of barium ferrite at dynamic shocked conditions](#)”, *J. Mat. Sci.: Materials in Electronics* **32**, 2429 (2021).
11. **S. Chakraborty**, G. Mulas, M. Rapacioli, and C. Joblin, “[Anharmonic Infrared Spectra of Thermally Excited Pyrene \(C<sub>16</sub>H<sub>10</sub>\): A Combined View of DFT-Based GVPT2 with Anharmonic CaOs, and Approximate DFT Molecular dynamics with DemonNano\\*](#)”, *J. Mol. Spectrosc* **387**, 111466 (2021).
10. G. Mulas, **S. Chakraborty**, “[Modelling anharmonic spectra of Polycyclic Aromatic Hydrocarbons at high temperatures](#)”, *Memorie della Società Astronomica Italiana* **91**, 291 (2021).
9. **S. Chakraborty\***, K. Demyk, Ludovic Biennier and R. Georges\*, “[Absorption Spectroscopy of Solid-Phase C<sub>60</sub> Fullerene between 1.65 and 2.78 μm\\*](#)”, *ACS Earth and Space Chemistry* **4**, 1540-1548 (2020).
8. B. Behera and **S. Chakraborty\***, “[Gas phase infrared spectra of H-bonded oligomers of methanol](#)”, *Vib. Spectrosc.* **106**, 102981 (2020).
7. K. Acharyya, S. Bhattacharyya, H. Sepehrpour, **S. Chakraborty**, S. Lu, B. Shi, X. Li, P. S. Mukherjee and P. J. Stang, “[Self-Assembled Fluorescent Pt\(II\) Metallacycles as Artificial Light-Harvesting Systems](#)”, *J. Am. Chem. Soc.* **141**, 14565-14569 (2019).
6. **S. Chakraborty**, G. Mulas, K. Demyk and C. Joblin, “[Experimental Approach to the Study of Anharmonicity in the Infrared Spectrum of Pyrene from 14 -723K](#)”, *J. Phys. Chem. A* **123**, 4139-4148 (2019).
5. **S. Chakraborty\***, S. Mukherjee, S. Mahapatra and P. K. Das, “[Infrared spectral assignment of Pyrimidine and Pyrazine in the C-H stretching region by an Effective Spectroscopic Hamiltonian](#)”, *Vib. Spectrosc.* **99**, 196-203 (2018).
4. K. Acharyya, A. Chowdhury, B. Mondal, **S. Chakraborty** and P. S. Mukherjee, “[Building block dependent morphology modulation of cage nanoparticles and recognition of nitroaromatics](#)”, *Chem. A. Eur. J.* **23**, 8482-8490 (2017).
3. **S. Chakraborty\*** S. Banik and P. K. Das, “[Anharmonicity in the vibrational spectra of Naphthalene and Naphthalene-d8: Experiment and theory](#)”, *J. Phys. Chem. A* **120**, 9707-9718 (2016).
2. **S. Chakraborty**, P. Das, S. Manogaran and P. K. Das, “[Vibrational spectra of fluorene, 1-methylfluorene, 1,8-dimethylfluorene](#)”, *Vib. Spectrosc.* **68**, 162-169 (2013).
1. **S. Chakraborty**, P. Das and P. K. Das, “[Isomeric identification of methylated naphthalenes using gas phase infrared spectroscopy](#)”, *Ind. J. Phys.* **86**, 209-218 (2012).

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