



Prachi Pandey

Curriculum-Vitae

OBJECTIVE

I have a Ph.D in Quantum dynamics with strong background in FORTRAN programming, electronic structure and vibronic coupling coputations. I am keen to apply my computational and theoretical expertise to address practical challenges in real-world chemical and materials systems. I seek a research position where I can contribute meaningfully to cutting-edge research aligned with the goals of the group and the focus of the advertised role.

RESEARCH EXPERIENCE

Doctoral Research (July,2016-March,2023)- University of Hyderabad, India

- Theoretical development of methods and tools for system-bath approach to nonadiabatic dynamics (NAD) and application to realistic molecular systems.
- Development of multireference methods
- Extensive programming in FORTRAN
- Teaching Assistant for 'Computer Applications and Programming Lab' course taught in the second year of M.Sc. Chemistry
- Teaching Assistant in 'Winter School for Gaussian' organized by the School of Chemistry, University of Hyderabad

Postdoctoral Research (June,2023-March,2024)- University of Hyderabad, India

- Theoretical development of path-integral techniques for quasi-potential landscape in quantitative biology
- Programming in MATLAB and FORTRAN and running computations requiring high-performance computing on clusters

Postdoctoral Research (June,2024-June,2025)- CNR-ICCOM, Pisa, Italy

- Development of Linear Vibronic Coupling (LVC) and Multi-Configurational Time-Dependent Hartree (MCTDH) protocol for theoretical simulation of quantum dynamics using Entangled Two-Photon Absorption (ETPA)
- Running LVC computations using OVERDIA code and FCClasses code
- Electronic structure calculations using Gaussian16 software

EDUCATION

2016-2023

PhD (Chemistry)
School of Chemistry, University of Hyderabad, India
Advisor: Prof. M. Durga Prasad
Thesis: **Studies on Nonadiabatic Dynamics within System-Bath Framework**

2012-2014

M.Sc (Chemistry)
Ramjas College, University of Delhi, India
Result: First Division

2009-2012

B.Sc (H) (Chemistry)
Miranda House, University of Delhi, India
Elective: Mathematics and Physics
Result: First Division

PUBLICATIONS

- **Prachi Pandey and M. Durga Prasad**, "Criteria for the Classification of System and Bath Variables in Nonadiabatic Dynamics: Application to Pyrazine", *J. Phys. Chem. A*, 2023, **127** (15), 3412–3426
- **Prachi Pandey and M. Durga Prasad**, "Time-Dependent Multireference Coupled-Cluster Method (TDMRCCM) for the Bath-Dynamics in System-Bath Approach to Nonadiabatic Dynamics", *J. Phys. Chem. A*, 2024 **128** (29), 5990-5998

CONFERENCES

1. National Conference of ICSC Spoke 7, Materials & Molecular Sciences
Organiser: ICTP, Trieste, Italy
Poster Presentation
May, 2025
2. 15th Symposium on Computing π -Conjugated Compounds
Organiser: University of Siena and CNR-ICCOM, Pisa
Poster Presentation
February, 2025
3. Structure and Dynamics: Spectroscopy and Scattering (SDSS-2023)
Organizer: IACS Kolkata, India
Poster presentation
October, 2023
4. 17th Theoretical Chemistry Symposium (TCS-2021) (Virtual)
Organizer: IISER Kolkata, India
Poster presentation
December, 2021
5. DAE Symposium on Current Trends in Theoretical Chemistry (CTTC-2020) Virtual
Organizer: Bhabha Atomic Research Centre, Mumbai, India
Poster presentation (Best Poster award)
September, 2021
6. CHEMFEST-2021 (18th annual in-house symposium)
Organizer: School of Chemistry, University of Hyderabad, India
Oral presentation
March, 2021
7. International Conference on Structure and Dynamics of Molecular and Condensed Matter Systems, ICSD-2020 (Held at Puri, Odisha)
Organizer: IISER Kolkata, India
Participation
March, 2020
8. 17th Conference on Spectroscopy and Dynamics of Molecules and Clusters,
Organizer: BITS, Pilani and IIT, Jodhpur (Held at Kumbhalgarh, Rajasthan)
Poster presentation
February, 2020
9. **Symposium on "Machine Learning for Science"**
Organizer: CCNSB, IIIT-Hyderabad
Participation
November, 2019
10. CHEMFEST-2019 (16th annual in-house symposium)
Organizer: School of Chemistry, University of Hyderabad, India
Poster presentation
February, 2019

SKILLS

- Programming languages: Fortran and MATLAB
- Computations using Gaussian16
- OVERDIA and FCClasses code
- Strong verbal and written communication skills in English

REFERENCE-CONTACTS

Prof. M. Durga Prasad
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Prof. Susanta Mahapatra
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DICHIARAZIONI SOSTITUTIVE DI CERTIFICAZIONI

(art. 46 D.P.R. n. 445/2000)

DICHIARAZIONI SOSTITUTIVE DELL'ATTO DI NOTORIETÀ

(art. 47 D.P.R. n. 445/2000)

la sottoscritta

COGNOME PANDEY

NOME PRACHI

NATO A: Lucknow, Uttar Pradesh

IL 24/12/1990

ATTUALMENTE RESIDENTE A:

INDIRIZZO

CAP

NAZIONE

Visto il D.P.R. 28 dicembre 2000, n. 445 concernente "T.U. delle disposizioni legislative e regolamentari in materia di documentazione amministrativa" e successive modifiche ed integrazioni;

Vista la Legge 12 novembre 2011, n. 183 ed in particolare l'art. 15 concernente le nuove disposizioni in materia di certificati e dichiarazioni sostitutive (*);

Consapevole che, ai sensi dell'art.76 del DPR 445/2000, le dichiarazioni mendaci, la falsità negli atti e l'uso di atti falsi sono punite ai sensi del Codice penale e delle leggi speciali vigenti in materia, dichiara sotto la propria responsabilità:

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comprensivo delle informazioni sulla produzione scientifico/tecnologica
corrisponde a verità

FIRMA