

**NATIONAL INSTITUTE OF TECHNOLOGY DURGAPUR  
DEPARTMENT OF CHEMISTRY**

Advertisement No. PROJECT-SG-NSM/2021, dated 08.04.2021

**RESEARCH ASSOCIATE (RA) at Department of Chemistry, NIT Durgapur**

**PROJECT: "Structure elucidation of simple hydrocarbons through Global Optimization using Density Functional Theory and post HF methods"**

**Principal Investigator:** Dr. Subhas Ghosal, Assistant Professor, Dept. of Chemistry, NIT Durgapur  
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**Co-Principal Investigator:** Dr. Anoop Ayyappan, Associate Professor, Dept. of Chemistry, IIT Kharagpur, Email: [anoop@chem.iitkgp.ac.in](mailto:anoop@chem.iitkgp.ac.in)

**Funding Agency:** DST, Government of India under National Supercomputing Mission (NSM)

**Duration:** Two years.

**Project Summary:** Hydrocarbons are an important in astrochemistry and astrobiology, in addition to being an integral part of life on Earth. While the stable hydrocarbon molecules found on Earth can be easily characterized with the current techniques, the transient hydrocarbons, especially in the interstellar medium and extreme conditions, are elusive. Using HPC facilities, we plan to develop a database of several isomeric geometries of all combinations of n and m in C<sub>n</sub>H<sub>m</sub> up to the practically affordable size. We will use an *Aufbau* approach of building up the molecules from C and H atoms, adding one atom at a time. For exploring this chemical space, we plan to improve the efficiency of our software, PyAR, by making it parallel and by adding more global optimization algorithms. The database of optimized geometries and other properties can be useful in identifying species in ISM and to understand the transient species during reactions.

**Qualification for RA:** (i) Motivated PhD holders in (theoretical) Chemistry or Physics from a recognized University/Institute within last two years (preferable).

**Desirable Experience:** Candidates should be well versed with

1. Coding in Python/Fortran/C language under HPC cluster environment.
2. Thorough with DFT and electronic structure calculation software e.g. ORCA, Gaussian, CFOUR, MOLPRO etc
3. Numerical methods of global optimization and other similar techniques.

**EMOLUMENTS:** (i) Total fellowship Rs. 47,000/- per month (consolidated) for the first year and Rs. 49,000/- per month (consolidated) in the second year after successful assessment by the review committee.

**HOW TO APPLY:**

The application email should contain the subject "NSM-RA Application". The application should include a cover letter and CV of the applicant.

**Mode of selection:**

Only short-listed candidates will be notified through email. No TA/DA will be paid for attending the interview. Online interview is also possible.



**Last date of application: 21.04.2021.**  
**Date of interview: 27.04.2021 (tentative)**  
**Date of Joining/start Date: 01/05/2021 (tentative)**

**TERMS & CONDITION:**

The above position is purely contractual. The selected candidate will not be entitled to claim for regular appointment/absorption in this Institute. Candidate has to devote full time to carry out the project. Other terms and condition will be as per those of NIT Durgapur.

*Subhas Ghosal*  
(Subhas Ghosal) 8/4/21

**Dr. Subhas Ghosal**  
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