

NATIONAL INSTITUTE OF TECHNOLOGY DURGAPUR
DEPARTMENT OF CHEMISTRY

Advertisement No. PROJECT-SG-NSM/2021/2, dated 26.07.2021

Junior Research Fellow (JRF) 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

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_nH_m up to the practically affordable size.

Qualification for JRF: (i) Motivated students holding MSc in Chemistry from a recognized University/Institute, preferably having physical chemistry specialization. Results awaited students may also apply, but salary will be as per DST norms if selected. (ii) The candidate must have qualified GATE or CSIR-UGC NET (including lectureship) in Chemistry examination.

Desirable Experience: Candidates should be well versed with

1. Coding in Python/Fortran/C language under Linux environment.
2. Thorough with the concepts of DFT and electronic structure calculations, Numerical methods of global optimization and other similar techniques.

EMOLUMENTS: (i) Total fellowship Rs. 31,000/- per month (consolidated)

HOW TO APPLY:

The application email (subhas.ghosal@ch.nitdgp.ac.in) should contain the subject "NSM-JRF 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: 08.08.2021.

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 26/7/21
(Subhas Ghosal)

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