# OFFICE OF INDUSTRIAL CONSULTANCY AND SPONSORED RESEARCH



## INDIAN INSTITUTE OF TECHNOLOGY MADRAS CHENNAI – 600 036

Advertisement No.: ICSR/PR/Advt. 138/2023 Dated: 02/08/2023

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Applications are invited for the temporary post of **Project Associate** in the Department of Chemical Engineering at IIT Madras for a project titled 'Development of protocols and machine learning potentials for investigation of liquid phase hydrodeoxygenation of polyols on complex catalysts.

**Co-ordinator:** Prof. Jithin John Varghese, Department of Chemical Engineering, IIT Madras.

**Duration:** Initially for six months and extendable upon positive review and recommendation by the review committee.

**Number of Vacancies: 01** 

S.No	Post	Qualification and Experience	Pay
1	Project Associate	Minimum Qualifications:  B. Tech / BE (Chemical/Materials/Metallurgical Engineering) or MSc (Chemistry/Physics) with an aggregate 70% marks or CGPA of 7.5 and higher in all degree programs. Prior experience in DFT simulations or molecular dynamics simulations or machine learning is a must and proficiency in coding/scripting is desirable.	Rs 27,000/- Per month

#### **Project Description:**

• This phase of the project is specifically targeted at developing computational workflows and reactive machine learning potentials (RMLP) which will enable carrying out reactive molecular dynamic's simulations of complex mixtures of the prototypical biomass derivatives and their hydrodeoxygenation products in aqueous medium, together with a multicomponent catalyst. Detailed DFT simulations and short duration Ab Initio MD simulations will be performed to generate the training data for developing the RMLP. The developed RMLP will be used for performing MD simulations of the reaction mixtures. The overall project is aimed at identifying catalytic performance and product selectivity descriptors for hydrodeoxygenation reactions on multicomponent catalysts. This is a crucial step in moving towards a bio-based specialty chemicals economy, replacing the conventional fossil fuel supply chains.

#### Job Scope:

• The job scope for this position will include (but not restricted to) survey and summarising of the literature, carrying out Density Functional Theory simulations of multifunctional catalyst, polyols and their hydrodeoxygenation products which are interacting with the catalyst, carrying out ab initio molecular dynamics simulations containing the relevant components described earlier, identifying and implementing appropriate machine learning framework to generate reactive potentials or forcefields using the DFT and MD data, data analysis, curating and reporting, contributing to scientific communication in the form of journal articles, technical reports and so on.

#### Note:

• Interested candidates may send his/her CV to **jithinjv@iitm.ac.in** with a brief letter of motivation and fit for the position.

The last date for submission of online application is 14.08.2023.

### **General Instructions to the candidates**

- 1) All the positions are on purely contract basis.
- 2) The completion of the period of contract will not confer any right for further extension, regularization, permanency at the Institute.
- 3) Candidates should apply online only in the website <a href="https://icandsr.iitm.ac.in/recruitment/">https://icandsr.iitm.ac.in/recruitment/</a> (Please check the advertisement number Advt. 138/2023 displayed and submit the application for the relevant position).
- 4) Separate application has to be filled for each post.
- 5) The system will accept single application only with the registered login ID (email) for an advertisement, hence the candidate is requested to select the multiple positions (In case, the candidate wishes to apply for more than one position) before the submission of application.
- 6) The application cannot be edited, reverted once it is submitted.
- 7) Candidates should not attempt to apply twice for the same post. If multiple applications are received from a candidate for the same post, the candidature will liable to be rejected.
- 8) Candidates should follow the prescribed procedure for submission of online application.
- 9) Candidates are advised to fill their correct and active e-mail addresses in the online application as all correspondence will be made by the Institute through e-mail only.
- 10) The candidates applying for any post should ensure that they fulfil all the eligibility conditions for the post. Their admission to any stage of the selection process will be purely provisional subject to confirmation that they satisfy the prescribed eligibility conditions. Mere issue of registration certificate / call letter to the candidate will not imply that the candidature has been found eligible.

- 11) After successful online submission of application, a printout of the application form must be obtained and submitted when called for test. It will be required at the time of document verification/test/interview. Hard copy of the application is NOT to be sent to the Institute.
- 12) Candidates must be citizens of India. Persons who have migrated from Pakistan with the intention of permanently settling in India or subjects of Nepal are also eligible, but in their case a certificate of eligibility from the Government of India will be necessary for appointment. Such candidates should apply to the Government of India in the Ministry of Home Affairs for necessary certificate and furnish satisfactory proof of having so applied.
- 13) The prescribed qualifications are minimum and unless specified, they are required for consideration for the post, even if higher qualification has been acquired and the mere fact that a candidate possesses the same will not entitle them for being called for interview.
- 14) Relevant experience gained after the minimum qualifying degree will only be taken into consideration. Minimum requirements of qualifications and/or experience can be relaxed in respect of exceptionally outstanding candidates.
- 15) The experience required is relaxable at the discretion of the Institute in the case of candidates belonging to the Scheduled Caste / Scheduled Tribe, if at any stage of selection the competent authority is of the opinion that sufficient number of candidates from these communities possessing the requisite experience are not likely to be available to fill up the vacancy reserved for them.
- 16) The Institute reserves the right to restrict the number of candidates for written / skill test / interview to a reasonable limit on the basis of qualifications, level and relevance of experience higher than the minimum prescribed in the advertisement and other academic achievements. The Institute also reserves the right of rejecting any or all the applications without assigning any reasons therefore.
- 17) Calling a candidate for test/interview merely indicates that it is felt that the candidate with others may be suitable for the post and conveys no assurance whatsoever that they will be recommended or selected or thier conditions specified in the application will be accepted.
- 18) Candidates will be short-listed for Test/Interview on the basis of the information provided by them in their online applications. They must ensure that such information is true. If at any subsequent stage or at the time of Test/Interview any information given by them or any claim made by them in their online applications is found to be false, their candidature will be liable to be rejected.
- 19) The Institute shall verify the antecedents or documents submitted by a candidate at any time at the time of appointment or during the tenure of the service. In case, it is detected that the documents submitted by the candidates are fake or the candidate has clandestine antecedents/background and has suppressed the said information, then their services shall be liable to be terminated.
- 20) In case of any inadvertent mistake in the process of selection which may be detected at any stage even after the issue of appointment letter, the Institute reserves the right to modify/ withdraw/ cancel any communication made to the candidates.

- 21) Applicants who are working in **any one of the Project at IIT Madras**, must apply through proper channel otherwise they will be required to produce No-Objection Certificate at the time of document verification/Test/Interview. Candidates without NOC will not be permitted to appear for Test/Interview.
- 22) Candidates may send testimonials from persons intimately acquainted with their work and character. If the applicant is in employment, the candidate should submit testimonials from the most recent employer or immediate superior as a referee.
- 23) The Institute has a right to decide the mode of screening and testing the applicant for short listing and selection.
- 24) The Institute solely reserves the right not to fill any advertised position without assigning any reason
- 25) Only shortlisted applicants will be contacted.
- 26) No correspondence whatsoever will be entertained from candidates regarding conduct and result of test/interview and reasons for not being called for interview. Canvassing in any form will be a disqualification.
- 27) The crucial date for determining the eligibility criteria for all candidates in every respect shall be the prescribed closing date for submission of online application.
- 28) The Institute strives to have a workforce which reflects gender balance and women candidates are encouraged to apply.
- 29) Any corrigendum/clarifications on this advertisement, if necessary, shall be uploaded on website and no separate communication will be sent for this purpose.
- 30) If there is any issue to submit the application please send E-mail to : recruitment@imail.iitm.ac.in / icsrrecruitment@iitm.ac.in Contact: 044- 2257 9796 on all working days from 9.00 AM to 05.30 PM (Monday to Friday except National Holidays). (Please note, only technical issues will be accepted No interim correspondence with reference to the selection process will be considered).
- 31) **Instructions to apply online:-**Eligible applicants would require to register and apply online through <a href="https://icandsr.iitm.ac.in/recruitment/">https://icandsr.iitm.ac.in/recruitment/</a> and submit the application.

Sd/-

Senior Manager –HR Centre for IC&SR IIT Madras