Recruitment for Postdoctoral Researcher

1. Position

・Job type: Specially Appointed Research Fellow
・Division: Global Collaborative Research and Education Center for Integrated Flow Science (IFS-GCORE)
・Number of Positions: 1

2. Job Description/ Field of Specialization

We are seeking a postdoctoral researcher to contribute to cutting-edge research at the intersection of quantum chemistry, combustion kinetics, and artificial intelligence. The goal of the project is to generate high-fidelity databases of temperature- and pressure-dependent thermochemical and kinetic properties of large, flexible, and radical species relevant to combustion and atmospheric chemistry. These databases will be used to develop and train AI/ML models capable of predicting rate constants and thermodynamic functions for species and reactions that are currently poorly understood or computationally inaccessible.
Key responsibilities include:

- Performing large-scale quantum chemical calculations to characterize potential energy surfaces and conformer distributions.
- Computing thermodynamic properties and pressure-dependent rate constants using advanced statistical mechanics and transition state theories, including multi-structural torsional anharmonicity.
- Developing curated datasets for training machine learning models (e.g., ANN, SVR).
- Assisting in the implementation of ML-based prediction tools for combustion chemistry applications, particularly for alternative fuel blends (e.g., ammonia-alcohol, ammonia-hydrocarbon systems).

This position will support the development of a robust and predictive framework for the design of next-generation sustainable fuels using theory-driven and data-driven approaches.

3. Required Qualifications and conditions:

- Applicants must hold a PhD in Theoretical/Computational Chemistry, Chemical Engineering, Physical Chemistry, or a related discipline.
- Strong background in quantum chemistry methods (e.g., DFT, MD, ab initio calculations) and software packages such as Gaussian, Polyrate, MultiWell, and MSTor is required.
- Familiarity with rate theory (e.g., RRKM, VTST, master equations) and statistical mechanics calculations is essential.
- Experience in modeling pressure-dependent reaction kinetics and conformer-resolved thermochemistry.
- Demonstrated skills in developing or applying machine learning algorithms (ANN, SVR) in molecular sciences are highly desirable.
- Proficiency with molecular descriptor generation tools (e.g., AlvaDesc, Dragon) and molecular data handling (e.g., SMILES, InChI) is advantageous.
- Strong programming and scripting abilities (e.g., Python, Fortran, MATLAB) are expected.

- Ability to work in a multidisciplinary environment and contribute to collaborative research efforts.

4. Starting Date and Conditions of Employment

As early as possible after July 2025

・Type of Contract: Full-time, fixed-term contract

・Term: Renewed each fiscal year. Maximum period is March 31, 2030

・Probationary Period: 6 months.

5. Salary and Benefits:

・Annual Salary: to be determined in accordance with Tohoku University's employment regulations. Approximately 5,000,000-6,000,000 JPY per annum. Allowances for transport may be provided depending on circumstances.

・Insurance: Admission into the MEXT Mutual Aid Association; provision of unemployment insurance and worker's accident insurance

・Working Hours:

The discretionary labor system for professional work shall apply. Flexible Work Hours: The standard working hours are 8:30 – 17:15, but the actual working hours are at the discretion of each employee.

Holidays: Saturdays, Sundays, National Holidays, New Year's Holidays (Dec. 29 - Jan. 3)

6. Application deadline and required documents

・Deadline: Until filled

・Requested Documents :

I. Curriculum Vitae with photo

Postal address and email address should be included.

II. A list of research achievements (original papers, proceedings, books and commentaries, presentations at national and international conferences, patents, competitive grants received, etc.)

III. Electronic files in PDF format of three selected papers.

IV. Summary of research achievements (A4 1 page)

7. Application Method

All documents must be submitted in PDF format via the following form:

[URL] https://docs.google.com/forms/d/e/1FAIpQLSchX9qzdMEnoj-4xbTQdgL6QcGsWTfhbDT_ijvIxLgvnCyNXQ/viewform?usp=header

If you experience technical difficulties with the online form, you may submit your application materials by email to the address below. In such cases, please use the subject line: "Postdoctoral Fellow Application – [Your Full Name]".

Email for alternative submission: [mani.sarathy@tohoku.ac.jp]

Note: Submitted materials will not be returned. Personal information will be used solely for the purpose of this recruitment.

8. Selection Process

Selection Process: After document review, an online interview will be conducted. Details of the interview will be communicated via e-mail.

Result: You will be notified of the screening results by e-mail.

For more information on the Institute of Fluid Science, visit:
https://www.ifs.tohoku.ac.jp/