

# **Open call for commissioned research project**

**Indo-Korea Science and Technology Center, Korea Institute of Science and Technology (KIST)**

Control number: IKST/Research/2022-01/03082022

**Indo-Korea Science and Technology Center (IKST), Bengaluru calls proposals for commissioned research project as below:**

## **1. Classification: Research & Development (Data analytics & experimental methods)**

No.	Field	Title of project	Budget	Period	Note
1	Research	Ab-initio modeling of materials using real-space based finite-elements at extreme-scale	Rs. 15,00,000/-	01/09/2022 to 31/08/2023	

## **2. Qualification and application**

A. Qualification for application

- ① Ph.D. degree holder in related area

B. Period of tender: **05.08.2022 (Friday) ~ 30.08.2022 (Tuesday)**

C. Required documents

- ① Official letter (one copy, English)  
② Project proposal (original two copies, English)

※ Email submission of above documents is mandatory to IKST HR (8046697004, [hr@ikst.res.in](mailto:hr@ikst.res.in), [ikst.admin@ikst.res.in](mailto:ikst.admin@ikst.res.in)), parallel with direct or postal submission

D. Application

● **Deadline: 17:30, 19.08.2022 (Fri)**

● **Submission (Direct or Post)**

- Address: NCC Urban Windsor, 3<sup>rd</sup> Floor, New Airport Road, Near Allalasanra gate, Opposite Jakkur Aerodrome, Bengaluru, Karnataka, India 560 065

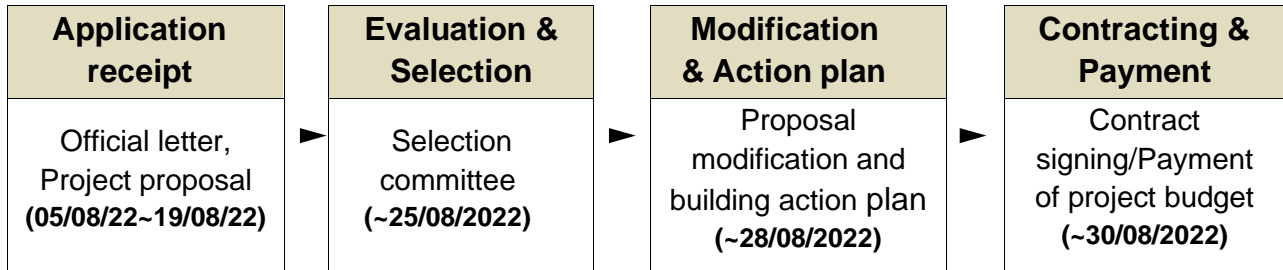
※ Please contact IKST HR (8046697004, [hr@ikst.res.in](mailto:hr@ikst.res.in)/ [ikst.admin@ikst.res.in](mailto:ikst.admin@ikst.res.in)) for any enquiry

- Attachments: 1. Selection & Operation plan for research project  
2. Request for proposal  
3. Project proposal (format)  
4. Project result report (format). End.

# Selection and operation plan for research project

## 1. Selection procedure and criteria

### □ Selection procedure:



※ Selection procedure timeline is subject to changes depending on internal schedules

### □ Evaluation & Selection:

○ Method: Written and presentation evaluation

○ Criteria:

- Fundamental qualification of institute and P.I.
- Clarity of objectives, differentiation of performance strategy, feasibility of research contents against the budget
- Creativity and innovativeness of objectives and contents, application availability of research results

### □ Modification & Action plan:

- Modification and improvement of project proposal of final candidate
- Building an action plan such as interim review, regular meetings etc.

### □ Contracting & Payment:

- Signing a commissioned survey research contract
- Major conditions/terms of contract
  - Objectives/Contents In final project proposal
  - Contract period: **01/09/2022 ~ 31/08/2023 (1 year)**
  - Payment: Advance (Inclusive tax, 100% of contracted amount, payment after contracting)

## **2. Result report**

- Result reports (original two copies) submission within two months from the last date of research period.

## **3. Notice**

- Selection result will be announced through email to individual(s)
- Duration for presentation evaluation is for 30 minutes (20 minutes for presentation and 10 minutes for Q&A)
- No documents will be returned after submission

# Request for proposal (RFP)

## **Ab-initio modeling of materials using real-space based finite-elements at extreme-scale**

DFT-FE (Density functional theory with finite elements) is a real-space method relying on an adaptive finite-element discretization that handles pseudopotential and all-electron calculations in the same framework and incorporates scalable and efficient solvers for the solution of the Kohn-Sham equations. DFT-FE is shown to handle periodic, semi-periodic, and non-periodic boundary conditions and general geometries. It is demonstrated to run on massively parallel many-core CPU and hybrid CPU-GPU architectures (tested up to ~200,000 cores on many-core CPUs and ~24,000 GPUs on hybrid CPU-GPU architectures) with excellent scalability. DFT-FE is currently capable of fast and accurate large-scale pseudopotential DFT calculations, reaching 50,000-100,000 electrons (about 5000 to 10000 atoms). The proposed project will involve the development of new computational methodologies to extend the DFT-FE capabilities and leverage the power of DFT-FE to address complex ab-initio material modeling problems which were not possible before.

# **Project Proposal** (Arial, Bold, 18 pt)

(Paragraph spacing 1.15)

## **1. Overview of project** (Arial, Bold, 12pt)

- Title (Arial, 12pt)
- Period
- Budget

## **2. Information of P.I.**

- Name:
- Affiliation: Position, Dept., Name of Institute
- Educational qualification:
- Contact
  - Tel.:
  - Mobile:
  - Email:

## **3. Necessity and objectives** (Max. 1 page)

## **4. Details** (Max. 3 pages)

## **5. Strategies, methods and system**

## **6. Expected achievements and application plan**

## **7. Deliverables**

## **8. Timeline**

## **9. List of participants and budget plan**

# **Project Result Report** (Arial, Bold, 18 pt)

(Paragraph spacing 1.15)

## **1. Overview of project** (Arial, Bold, 12pt)

- Title (Arial, 12pt)
- Period
- Budget

## **2. Information of P.I.**

- Name:
- Affiliation: Position, Dept., Name of Institute
- Educational qualification:
- Contact
  - Tel.:
  - Mobile:
  - Email:

## **3. Objectives** (Max. 1 page)

## **4. Details** (No limit of pages)

### **4.1 Introduction**

### **4.2 Methods**

### **4.3 Results**

### **4.4 Conclusion**

## **5. Deliverables**

## **6. Expenses**