Machine learning from computational materials science data for modelling nanocrystal catalysts

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# 2<sup>nd</sup> Call for Virtual Mobility (VM) Grants for activities occurring between April 1<sup>st</sup> and August 31<sup>st</sup>, 2025

COST Innovative Grant 18234: Machine learning from computational materials science data for modelling nanocrystal catalysts (NanoCatML) is under COST, an EU-funded, intergovernmental framework for European Cooperation in Science and Technology.

This grant follows *COST Action 18234: "Computational materials sciences for efficient water splitting with nanocrystals from abundant elements".* 

COST Actions offer an open space for collaboration among scientists across Europe (and beyond) and thereby give impetus to research advancements and innovation.

For more information about COST IG18234, please visit our COST webpage: <a href="https://comp-h2o-split.eu">https://comp-h2o-split.eu</a>

### What is Virtual Mobility (VM) Grant?

Virtual Mobility consists of a collaboration in an **online setting** among researchers, innovators within the COST Action, to exchange knowledge, learn new techniques, etc. Virtual Mobility benefit to:

- <u>COST Action</u>: uses a flexible tool to implement online activities inside the network, achieve the MoU objectives and significantly increase their impact and reach. Contributes to European leadership in knowledge creation and increasing its innovation potential.
- <u>VM grantee</u>: develop(s) capacity in online collaboration and networking in pan-European framework.

# **Examples of activities that can be performed by VM grantee are:**

- Virtual mentoring scheme, with special focus on activities and exchanges that
  can generate capacity building and new skills, particularly for Young
  Researchers and Innovators (e.g. managerial skills, methodological skills,
  communication skills, etc).
- To support the harmonisation and standardisation of methods and procedures within the Action networking activities, e.g:
  - Setting up a survey amongst all Action members to collect different results and outcomes from experiments done in their respective labs and research groups.
  - Coordinating the discussions to create common protocols to be used by the network afterwards.
  - Preparing questionnaires and response scales to be used by the Action members as part of virtual networking activities.

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- To support the implementation of research coordination related activities that do not necessarily require in-person presence, e.g.
  - Computational or modelling activities.
  - Data analysis of the Action for a specific report or activity.

# **Applicants for VM Grants** can be individuals affiliated to a legal entity in:

- A COST Full/Cooperating Member
- An European RTD
- A NNC

Eligible VM Grant applicants must submit their VM Grant applications online at the following web address: <a href="https://e-services.cost.eu/grants">https://e-services.cost.eu/grants</a>

# Specific subjects targeted by COST IG 18234

COST IG 18234 invites applications for Virtual Mobility (VM) Grants on these subjects:

- ✓ Survey the type of frequently used codes for Machine Learning that involves data from computational materials science. Codes with specific emphasis on catalysis are preferred or any other useful code on electronic structure calculations that will contribute to the community.
- ✓ Survey available sources of data (NOMAD, Materials Genome, etc.) and collect information on the data that were calculated with different computational methods (density functional theory, molecular dynamics or Monte Carlo).
- ✓ Survey by type of data to collect, e.g. crystal structure, electronic properties (chemical bonding types, band gap, or band positions), catalytic overpotentials, kinetic properties (activation barriers or current-voltage simulation results).

#### **Financial support**

A VM Grant is a fixed financial contribution which takes into consideration the budget request of the applicant and the evaluation of the outcomes of the VM Grant.

The maximum amount per VM Grant is up to 1,500 €. Each VM Grant sum will be decided by the Core Group, based on the request of the applicant.

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Grants are paid by the Grant Holder after the completion of the activity and approval of all required report/documentation<sup>1</sup>.

### **Scientific report**

collaboration.

The grantee will perform the tasks in line with the approved application.

Once the activity has ended, the grantee will submit the required reports and relevant documentation in e-COST including: the work developed, main outcomes and achieved outputs of the Virtual Mobility, and description of the future follow up

The report will be submitted within 30 days after the end date of the activity or 15 days after the end date of the Grant Period, whichever comes first.

The VM Grants must be aligned with the general objectives of the COST Action 18234, which targets the understanding, design and fine tuning of material properties for energy conversion processes using computer simulation approaches toward a multiscale strategy.

### How to apply

VM activities must occur in their entirety within the dates specified in this call.

The applications are to be submitted no later than May 31st, 2025.

- 1. All applicants must register for an e-COST profile at <a href="https://e-services.cost.eu/">https://e-services.cost.eu/</a> adding their CV and bank account details to their profile.
- 2. All applicants must complete and submit their VM Grant application online at: <a href="https://e-services.cost.eu/grants">https://e-services.cost.eu/grants</a> using dedicated forms available
- 3. The application shall include:
  - Title of the activity
  - Start and end dates (within the current Grant Period)
  - Budget requested by the applicant.
  - The application form (available at the e-COST website) describing: (main) objective(s), description of the work to be carried out by the applicant, plan for participation, expected outcomes and description of the contribution to the MoU objectives.

The applications will be then assessed by the Grant Awarding Coordinator and the Core Group, against the perceived contribution that the proposed grant will make in

<sup>&</sup>lt;sup>1</sup> Financial support for networking activities organised through a Grant Awarding Process is a grant awarded to individuals, not intended to cover employment costs.

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accordance to the scientific objectives outlined in the Action Memorandum of Understanding (MoU).

Please note that COST can request additional information to substantiate the information contained within the documents submitted by VM Grant applicants.

Evaluation results will be communicated to the applicants within three weeks after the application submission.

Upon approval of the application, the Grantee receives a Grant Letter from the Grant Holder stating the approved amount and the conditions for receiving the grant.

COST Action reserves the right for justified reasons to leave the position open, to extend the application period and to consider candidates who have not submitted applications during the application period.

# For further details, please contact:

Dr. José Gomes, Grant Awarding Coordinator <u>jrgomes@ua.pt</u> Smadar Amir, Grant Manager <u>smadaram@technion.ac.il</u>

- ✓ Deadline for applications to be submitted: 31.5.2025
- ✓ You can apply any time until May 31<sup>st</sup> (Notification of application outcome will be sent three weeks after submission)
- ✓ Period of Virtual Mobility Grants: 1.4.2025 31.08.2025