NFDI4Solar

Letters of Intent

1 Binding letter of intent as advance notification or non-binding letter of intent

☐	Binding letter of intent (required as advance notification for proposals in 2020)
☒	Non-binding letter of intent (anticipated submission in 2021)

2 Formal details

- Planned name of the consortium
  Consortium for integrating efforts on solar energy conversion in photovoltaics, photoelectrochemical cells and solar fuels
- Acronym of the planned consortium
  NFDI4Solar
- Applicant institution
  [Martin-Luther-University (MLU) Halle-Wittenberg, Universitätsplatz 10, 06108 Halle (Saale)]
  [Name of the head of the institution: Prof. Dr. Christian Tietje]
- Spokesperson
  [Wouter Maijenburg, wouter.maijenburg@chemie.uni-halle.de, Martin-Luther-University (MLU) Halle-Wittenberg]

- Co-applicant institution
  [Ludwig-Maximilians University of Munich (LMU)]
  [Name of the head of the institution: Prof. Dr. Bernd Huber]
- Co-spokesperson
  [Tayebeh Ameri, tayebeh.ameri@lmu.de, University of Munich (LMU)]

Other co-applicants so far;

- Miguel Marques, miguel.marques@physik.uni-halle.de, MLU
- Roland Scheer, roland.scheer@physik.uni-halle.de, MLU
- Christian Hagendorf, Christian.Hagendorf@csp.fraunhofer.de, Fraunhofer Center for Silicon Photovoltaics (CSP)

[Please repeat for all co-applicant institutions/co-spokespersons within the planned consortium.]

- Participant

  So far, we have made the following list of possible co-applicants and participants and contact and agreements for detailed collaboration will be achieved in near future.

- Roel van de Krol, Helmholtz-Zentrum Berlin
- Radim Beranek, Ulm University
- Wolfram Jägermann, TU Darmstadt
- Bettina Lotsch, MPI for solid state research, Stuttgart
- Clemens Heske, Karlsruhe Institute of Technology (KIT)
- Thomas Unold, Helmholtz-Zentrum Berlin (HZB)
- Uli Lemmer, Karlsruhe Institute of Technology (KIT)
- Vladimir Dyakonov, Julius-Maximilians University of Würzburg (JMU)
- Barry Thompson, University of Southern California
- Maria A. Loi, University of Groningen
- Jenny Nelson, Imperial College London
- Henry J. Snaith, University of Oxford
- Alan Aspuru-Guzik, University of Toronto

3 Objectives, work program and research environment

- **Research area of the proposed consortium (according to the DFG classification system:**

307 Physik der kondensierten Materie

322 Chemische Festkörper- und Oberflächen-forschung

323 Physikalische Chemie

406 Material-wissenschaft

409 Informatik

- **Concise summary of the planned consortium's main objectives and task areas**

Harvesting solar energy is one of the most promising solutions towards a greener planet and better human welfare. Photovoltaics (PV) and photoelectrochemical (PEC) devices have been at the center of research in this field. However, the correct operation of these devices is governed by a set of complex multi-level phenomena from the quantum level, the mesoscale and interfaces, to the macro scale, process, and architecture. Three separate methodological approaches are currently employed for the development of such solar energy conversion

systems: A) Experimental material/device design of the complete PV/PEC systems, which involves iterative processing, characterization and modeling steps; B) Material screening for the complex semiconductor materials based on selected properties; and C) Theoretical simulation and modeling of the layer and interface subsystems based on atomistic models. However, to accelerate the workflow of material discovery, device design and deployment to the market, reciprocal communication between these three approaches is highly needed. Therefore, NFDI4Solar has the following objectives:

Objective 1: Iceberg!

A successful data mining trial or a well-trained (machine learning) algorithm needs a structured experimental data source that contains both **desired** and **undesired** scenarios. However, data reported in the scientific literature represents those desired results, while the undesired observations are rarely reported. On the other hand, the peer review process demands either the publication of new efficiency records compared to previous publications or a deeper insight into the functional systems. For example, in the field of organic photovoltaics, it is believed that only one-tenth of all the produced data are reported in the scientific journals, while the other precious (from a data scientist perspective) ninety percent is buried in the lab books. Knowing that there are around 20,000 ISI papers about organic photovoltaics and assuming an average of 3 sets of data records per paper, there are around half a million unpublished data records. This resembles an iceberg, in which the tip resembles those small shares of published data and all the unpublished data sets remain submerged under water. If we could collect a small part of this submerged data, this can already hugely help the AI models to learn the undesired situations and help them to decode the unknown multi-level structure-property relationships. Therefore, NFDI4Solar plans to collect the submerged data with the help of the most prominent scientists in the field; both on a national and an international level.

Objective 2: Device continuum

In recent years, many computational and theoretical studies have been done, and many databases and repositories have been constructed in the field of solar energy conversion devices and materials. However, they only focused on a specific part of these systems, which were mostly the materials in the active layer. Here, we plan to consider these devices on a multi-level scale from electronic properties to the device scale. Additionally, in order to understand the working principle of the entire device, special emphasis will also be given to solid-solid and solid-liquid interfaces.

Objective 3: A paradigm shift

One of the main goals of NFDI4Solar is to have an impact on the culture of research in the field of solar energy converters from just experimental or just theoretical to an integrated model of

experimental and theoretical. Enhancing communication between these two disciplines will accelerate the ongoing progress and lead to a faster realization of devices with higher efficiencies.

Objective 4: FAIR principles

Given the complexity of PV and PEC systems, correct implementation of the well-known FAIR principles is an essential step to guarantee the success of objectives 1 to 3.

To achieve the objectives mentioned above, NFDI4Solar will manage the following tasks areas.

Task Area 1: Infrastructure

A first step is to gather the community for collaborations. This contains the accurate determination of the ontology, terms and nomenclature for each subarea (Organic PV (OPV), Perovskite PV, PEC, dye-sensitized solar cells (DSSC), etc.) on a multi-level range. We will seek a machine that is capable to read the published reports and to fill the repository with unstructured data preliminarily. Then, supervision is needed to check the machine-fetched data, and the following steps will be constructed on the bedrock of this infrastructure.

Task Area 2: Collaborations and representatives

To meet objectives 1 and 3, we need a close connection with the community. This collaboration is divided into two main areas: first acquiring the previously collected non-published and/or current experimental data and instructing the collaborators to import them into the repository through the user interface, and second, presenting how our developed infrastructure can help the research in the preliminary designing steps, and during and after conducting the experiments. This task is divided into different subfields and length scales, as shown in Table 1. The co-applicants are selected in a way to cover all these subtasks, and they are in contact with international participants.

Table 1: Sub-tasks in task area 2.

		Scale		
		Quantum level	Meso- and Microscale (intra-molecular and interface level)	Macroscale (device architecture)
Fields	Photoelectrochemical cells and solar fuels	TA 2.1.1	TA 2.1.2	TA 2.1.3
	1st and 2nd generation solar cells (Silicon, CIGS, etc.)	TA 2.2.1	TA 2.2.2	TA 2.2.3
	3rd generation solar cells (Organic, Perovskite, DSSC, QDs, etc.)	TA 2.3.1	TA 2.3.2	TA 2.3.3

Task Area 3: Coordination and intra-consortia networking

The applicant institute is committed to organize the proposed project involving all aforementioned task areas and to establish the networking with other NFDI consortia looking for synergies in subsequent efforts. Figure 1 provides a schematic overview of the consortia's task areas inspired by the iceberg idea.

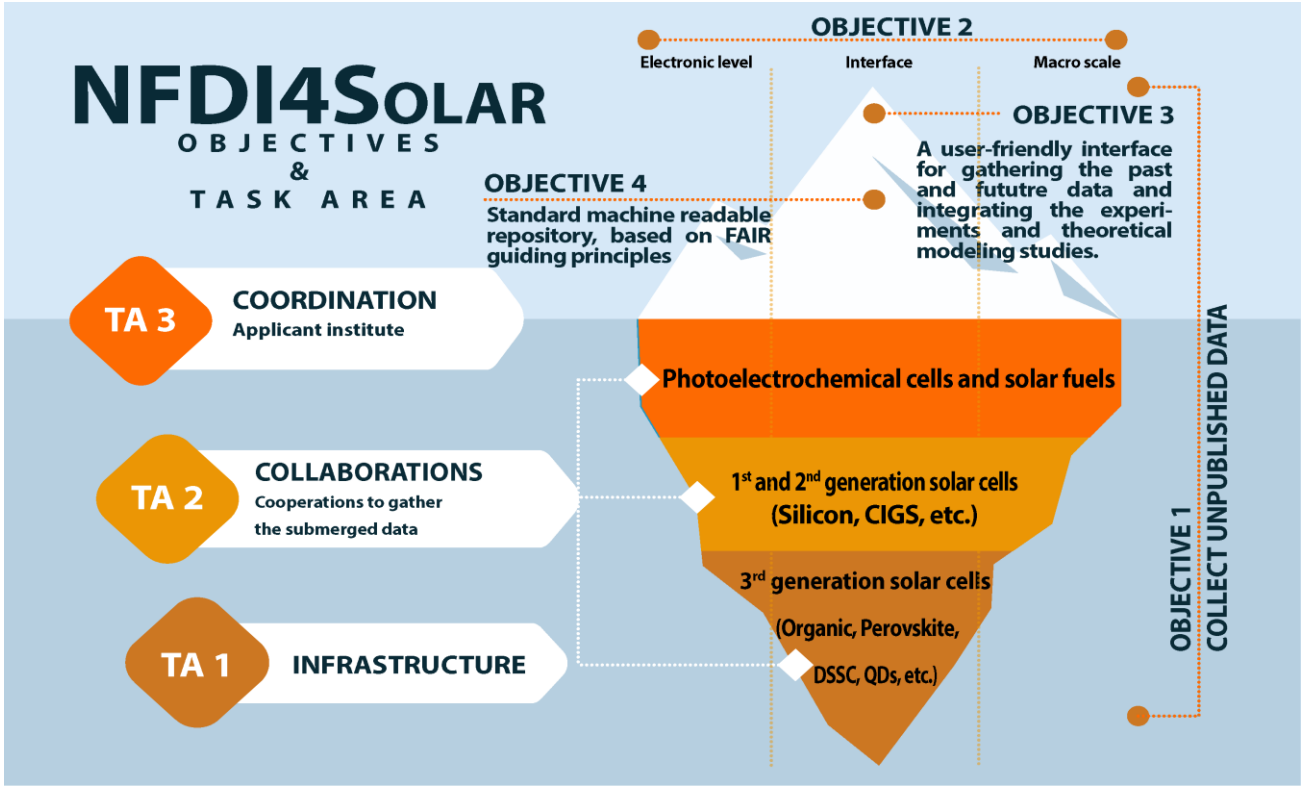

Figure 1: Schematic presentation of NFDI4Solar.

- **Brief description of the proposed use of existing infrastructures, tools and services that are essential in order to fulfil the planned consortium's objectives**

All the co-applicants are well-known in their related field. This reputation will help our success in the first objective, which eases cooperation with the international participants. Moreover, we have already generated a considerable amount of unpublished experimental data ourselves, which allows us to test and debug the beta version of the repository as well as AI outputs with supervised data points. This will help us persuade the community to get involved in the projects.

- **Interfaces to other proposed NFDI consortia: brief description of existing agreements for collaboration and/or plans for future collaboration**

The 2020 NFDI conference was very important for us as it provided the opportunity for the two groups (PEC and PV) to get in touch and team up, which illustrates that we are keen to further

expand our consortium through multilateral talks, conferences and negotiations. To keep the unity of procedures, ontology, metadata standards and other general cross-cutting topics, we will collaborate with all other NFDI initiatives. However, specific collaboration potentials can be found on the topic of multi-scale modeling (FAIRmat) as well as on the topic of materials interfaces (NFDI4Cat), which will both be pursued. Additionally, NFDI4chem addresses the digital lab book, which is an essential part of our project as well. Furthermore, cooperation with the engineering consortia (NFDI4Ing and NFDI4MSE) will synergistically promote our efforts on constructing infrastructures and high-throughput data management solutions. However, even though we can find synergies with several other NFDI consortia, we feel that we cannot merge with any of them, since neither of them provides a clear multi-disciplinary approach (combining physics and chemistry AND experiments and theory) AND addresses the importance of interfaces (solid-solid AND solid-liquid) AND addresses all phenomena taking place on multiple length scales (ranging from the electronic level to the macro scale), which are all indispensable for a successful integration of materials and devices for solar energy conversion into the NFDI initiative.

4 Cross-cutting topics

Please identify cross-cutting topics that are relevant for your consortium and that need to be designed and developed by several or all NFDI consortia.

- Best practice to encounter submerged data
- The involvement of international players
- FAIR data guidelines
- Infrastructure, repository, tools and related services
- Intellectual property and legal aspects
- Sustainability and lifetime of the infrastructure and collaboration established within the NFDI4Solar

- **Please indicate which of these cross-cutting topics your consortium could contribute to and how.**

General cross-cutting topics such as following the FAIR data principles and developing infrastructures as well as legal aspects of the data ownership are those common topics that will be faced by all consortia. Therefore, they are supposed to be considered throughout the wisdom of the crowd of specialists who are already involved in NFDI's consortia, and we will join them for specific customizations.

However, we will provide specific guidelines (best practice) related to submerged data. The concept of collecting unpublished data is potentially useful for all other consortia in any level of progression. Moreover, NFDI4Solar aims to persuade international institutions to a sustainable involvement in the project by different strategies, e.g., gamification. Sharing successful experiences in this field with other consortia will promote their progress as well.