HANAMI

HPC ALLIANCE FOR APPLICATIONS AND SUPERCOMPUTING INNOVATION: THE EUROPE - JAPAN COLLABORATION

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DELIVERABLE D6.1

Projects setup

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Version History

Revision	Date	Editors	Comments
0	16/08	Michele Casula	First version released to the Reviewers (WP6.5 incomplete, WP6.6 missing)

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1	23/08	Michele Casula	Implementation of suggestions from Daniele Varsano's review (WP6.5 still incomplete, WP6.6 still missing)
2	28/08	Michele Casula	All contributions are now included. The document is complete.
3	28/08	Michele Casula	Implementation of suggestions from Edoardo Di Napoli's review

Glossary of Terms

Item	Description
HPC	High Performance Computing
DFT	Density Functional Theory
QMC	Quantum Monte Carlo
MBPT	Many Body Perturbation Theory
PIMD	Path Integral Molecular Dynamics
NQE	Nuclear Quantum Effects

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Executive Summary

In WP6, HANAMI will address major societal and technological challenges via the conception and exploration of innovative solutions in the context of Materials Science. The work package 6 is carefully structured in a number of distinct projects such as, for instance, the study of lead-free perovskites for photovoltaics, electrochemistry and battery research from first principles, hydrogen storage and energetics, as well as the development of an abstract layer for applying linear algebra routines across different materials science codes. These projects will be realized by means of setting up, building and consolidating collaborations with Japanese partners, triggered and promoted by the HANAMI framework. A particular effort is planned to optimize the corresponding computational codes for both European and Japanese, pre-exascale and exascale-ready supercomputers. After this initial HANAMI period all WP6 tasks are up and running, also thanks to previously settled collaborations with Japanese partners that HANAMI will contribute to foster and further strengthen. These projects will be consolidated thanks also to the use of financial resources for hiring postdoctoral fellows, whose recruitment is at an advanced stage in most of the WP6 projects. Part of the allocated budget will also be spent for travelling to visit the Japanese collaborators by the HANAMI European members, who have already planned most of their trips.

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1. Introduction

In the quest to develop sustainable energy technologies, scientists and researchers have turned to computational tools to study and optimize various materials properties. The current and future evolution of High Performance Computing (HPC) enables new dimensions in materials design, especially in terms of increasing complexity of the accessible systems and properties, leading also to increased accuracy and improved approximations of the computational approaches. Combined with the increased high-throughput and materials informatics capacities, these advancements enable to address major societal and technological challenges in unprecedented ways that will be explored through this collaboration.

Both Japan and Europe have leading teams active in this domain. This WP aims at strengthening the collaboration between these groups through two main activities:

1. Selected research projects aimed at improving materials sustainability for applications relevant to energy production and storage (tasks 6.1, 6.2, 6.3);
2. Joint development efforts aimed at creating extremely scalable libraries and innovative software that may enable future frontier applications (tasks 6.4, 6.5, 6.6).

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2. Report on the initial setup of the projects and the building and consolidating of the collaborations with the Japanese partners

2.1 Task 6.1. Sustainable materials for photovoltaics. Task Leader: Giacomo Giorgi, CNR, Perugia

Brief summary of the project Within this task we plan to deploy and optimize the Many-Body Perturbation Theory (MBPT) first-principles code Yambo [A.Marini, C.Hogan, M.Grüning and D.Varsano, Comp. Phys. Comm. **180**, 1392 (2009); D. Sangalli *et al.* Journal of Physics: Condensed Matter **31**, 325902 (2019)] on Japanese supercomputers. We will optimize the code for the Fugaku architecture and conduct a series of benchmarks to fine-tune parameters for handling large systems. A particular attention will be devoted to the linear algebra solvers for the solution of the Bethe-Salpeter equation to calculate optical absorption spectra for system containing hundreds of atoms in their unit cells. This preliminary work is essential to estimate the resources required for calculations on the electronic and optical properties of lead-free perovskite systems. Given the size and complexity of the targeted systems, the Fugaku supercomputer will be instrumental in achieving these results. Subsequently, we will exploit Density Functional Theory (DFT) and MBPT to evaluate the photoconversion efficiency of lead-free and 2D perovskites and determine the impact of grain boundaries on their performance exploiting both Japanese and European supercomputers.

Description of the team The team is composed by Giacomo Giorgi (University of Perugia and CNR-Nano, Modena), Daniele Varsano (CNR-Nano, Modena), and Maurizia Palummo (University of Rome “Tor Vergata”) on the EU side. DV is in charge of optimizing the Yambo code for the Fugaku architecture. GG and MP are in charge of exploiting such optimization in order to calculate electronic and optical features of materials of interest (as mentioned, both 3D and 2D halide perovskites)
The Japanese side is formed by Prof. Koichi Yamashita (University of Tokyo and Yokohama City University) and Takahito Nakajima (RIKEN Center for Computational Science, RIKEN R-CCS). They are both in charge of the atomistic modelling from first-principles of materials for technological applications, with special focus on lead-free halide perovskites.

Recruitment and Resources In the framework of the project, a two-years postdoctoral fellowship has been announced, and we are confident that the position

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will be filled by fall 2024. The ideal candidate will be trait d'union among the parts involved in the task. Concerning the HPC resources needed to achieve the objectives, we have successfully applied for computational resources on Fugaku supercomputer. The project (project Yambo_Scale: hp240326, Trial Access Project) submitted jointly with the Japanese partners has already been granted. The necessary procedures for accessing the supercomputer, including identity verification and the statement of pledge, have been completed, and the accounts for all the team members have been created. We anticipate having access to the supercomputer and commencing the deployment and benchmarking campaign at the beginning of September 2024. In parallel, benchmarks will be also carried on on EuroHPC Leonardo supercomputer where computational resources have been already granted.

Collaboration strategy Given the longstanding collaboration with Prof. Yamashita, which includes Prof. Giacomo Giorgi and Prof. Maurizia Palummo's recent visit to Yamashita's group in July 2024 for a scientific exchange, we are planning to continue in the same direction. The strategy will involve scheduled reports on the common activity progress, organization and participation in workshop, and the continuous involvement of students and researchers in exchange activities. To further solidify this partnership, a joint bilateral project between CNR and JSPS, spanning two years (2025-2026), will be submitted at the beginning of September. This project will involve the European and Japanese partners of this task, with a key focus on the dissemination and training activities related to the Yambo code and its optimal usage on Japanese supercomputers. We plan to visit Prof. Yamashita group in Summer 2025, and 2026 under HANAMI support and the bilateral CNR/JSPS project if it will be successful.

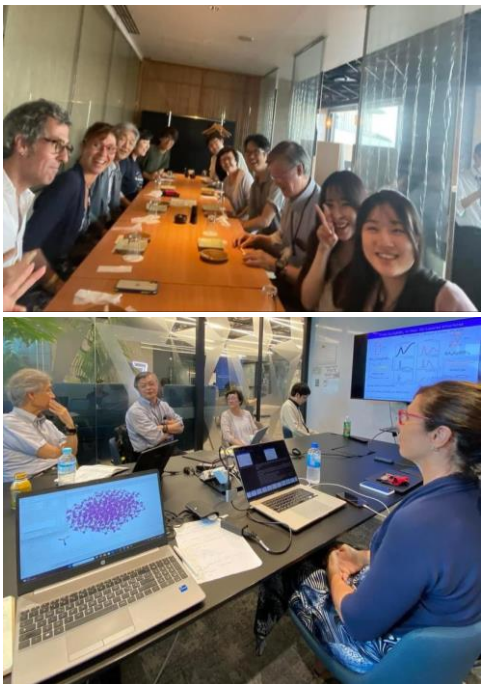

Figure 1: Pictures of the joint meeting with Yamashita's group in July 2024

2.2 Task 6.2. Electrochemistry and battery research from first principles. Task Leader: Pablo Ordejon, ICN2, Barcelona

Brief summary of the project In this task, we will collaborate on the development of methods based on DFT for the study of the electrochemical interface and battery materials. In particular, we aim at combining the DFT code SIESTA, developed by the group at ICN2 (Barcelona), with the Effective Screening Medium (ESM) package developed by the group of Minoru Otani in Tsukuba (Japan). The resulting software will be optimized on the EuroHPC and Japan pre- and exascale supercomputers. The software will be applied to several problems involving battery materials, and this work will be complemented with computational spectroscopy simulations performed with the Quantum Espresso [P. Giannozzi *et al.*, J. Chem. Phys. **152**, 154105 (2020)] and Yambo codes.

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Description of the team The team in Europe includes Pablo Ordejón and Jose María Escartin (ICN2, Barcelona), and Deborah Prezzi (CNR-Nano, Modena). PO and JME, together with a postdoc recruited by the project, will work on the connection of the SIESTA [J. Chem. Phys. **152**, 204108 (2020)] and the ESM codes, and its application to battery materials and electrochemistry problems. DP will collaborate on automated workflows for computational spectroscopy simulations.
The team in Japan includes Minoru Otani (University of Tsukuba) and Yoshitaka Tateyama (NIMS Tsukuba). MO will collaborate on the link between SIESTA and ESM, while YT will provide his expertise about battery materials and electrochemical problems as application cases of the developed codes.

Recruitment and resources A two-year postdoctoral position has been announced at ICN2 to work on this Task. The call was open in Spring 2024 (see https://jobs.icn2.cat/job-openings/621/postdoctoral-researcher-hanami-theory-and-simulation-group), and the final selection is taking place right now. The candidate chosen will start by September 2024.
Concerning the HPC applications to access to supercomputers, we already have been granted test projects in all the major EuroHPC computers, including Deucalion (Portugal), which has an architecture very similar to Fugaku. We will then use Deucalion as testing bed for the optimization of our software, and then apply for computational resources in Fugaku for fine-tuning.

Collaboration strategy The group led by Minoru Otani at the University of Tsukuba will provide the initial working versions of ESM and its interface to older versions of SIESTA, and will participate in the definition of the new, general and version-agnostic interface between SIESTA and ESM. They will also provide results to validate the new implementation and expertise in the use of Fugaku supercomputer, which they have been using for their research in batteries materials and electrolytes. Initial discussions between both groups have already been established.
Most of the work related to SIESTA in HANAMI will directly involve the Europe-Japan collaboration. The programming work will be managed by the ICN2 team (PO, JME and the postdoc hired by HANAMI), with continuous consultation with the Japanese team. While most of the testing of the developed codes will be conducted in European pre- and exascale machines, the tests will also be carried out in close collaboration with the Tsukuba team.

2.3 Task 6.3. Hydrogen storage: adsorption, desorption, reaction barriers from QMC. Task Leader: Michele Casula, CNRS, Paris

Brief summary of the project This task will be focused on the quantitative understanding of hydrogen and its chemistry in hydrogen-bearing systems, such as superconducting hydrides and hydrogen-hosting clathrate hydrates. Modelling hydrogen-mediated or hydrogen-involving interactions in a predictive way is a challenging problem because it requires an accurate evaluation of binding energies and a proper account of nuclear quantum effects (NQE). In this task we address both points by using Quantum Monte Carlo (QMC) as method of choice to evaluate the chemical binding energy, and the path integral molecular dynamics (PIMD) to take into account NQE. We will employ the TurboRVB code [K. Nakano *et al.*, The Journal of

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Chemical Physics **152**, 204121 (2020)], which has both capabilities, as it implements efficient QMC algorithms and it also includes a built-in PIMD code. More specifically, we plan to combine QMC with Machine Learning (ML) techniques to generate fast and accurate potential energy surfaces, and enhance the portability of TurboRVB towards HPC and its interoperability with existing ML software. This will be done also thanks to the recent deployment of TurboGenius, a workflow manager seamlessly interconnected with TurboRVB, and developed by Kosuke Nakano at NIMS, Tsukuba. The improved workflow will allow one to combine more easily the complex sequence of steps necessary to go from the creation of the first set of nuclear configurations, the QMC calculations of the electronic energies and nuclear forces, the ML-potential generation, and its final use in PIMD simulations. The developed workflows will be general, and runnable on different machines, in Europe as well as in Japan.

Description of the team The team is composed by Michele Casula, CNRS research director, working at the IMPMC laboratory of Sorbonne University, Paris, and by two postdocs, recently recruited on the HANAMI funding, namely Abhishek Raghav and Marco Cherubini. Dr. Kosuke Nakano, research scientist at NIMS, Tsukuba, coordinates the activities from the Japanese side.

Recruitment and Resources In the HANAMI framework, two years of postdoc have been allocated to this task. We rapidly proceeded to the recruitment of two postdoctoral fellows, filling a year contract each. They both started in May 2024, a couple of months after the official starting date of HANAMI. We believe that this parallel and early recruitments will boost the WP6.3 task in the first stages of development, necessary then to navigate towards more applied tasks with the needed tools already developed.
As far as the computational resources are concerned, we have been granted a common allocation in the Fugaku supercomputer, as regular access, as well as in the Leonardo pre-exascale computer, as benchmark access. The latter has been the preliminary step towards an extreme scale access application, already sent and now under review, and profoundly inspired by this HANAMI WP6.3 task. National French and Japanese allocations, regularly granted to the team members, will also be used to reach the goals of this task.

Collaboration strategy In the frame of HANAMI, we are developing a fruitful collaboration with Kosuke Nakano, research scientist at NIMS, Tsukuba. Our scientific cooperation has been active since many years. It was sparked by the development of the QMC TurboRVB code, and fostered by the previous European TREX project, aim at developing a European Center of Excellence in high performance computing addressing stochastic electronic structure methods. The TREX project ended a couple of months ago. HANAMI is going to be fundamental to consolidate this collaboration, by keeping it fruitful and interactive. HANAMI WP6.3 focusses on the development of a general QMC workflow for the MLPs generation, and it will benefit from Dr. Nakano's deep knowledge of the Fugaku architecture and Japanese HPC infrastructures. The resulting workflow manager will thus be optimized for both European and Japanese supercomputers. We are having weekly zoom meetings and frequent email exchanges to align on the workflow strategy development and on its applications. We plan to visit Dr. Nakano in spring 2025, under HANAMI support, and we already scheduled Dr. Nakano visit in Paris for September 2024, under Nakano's personal grant.

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2.4 Task 6.4. Numerical linear algebra framework for Materials Science. Task Leader: Edoardo Di Napoli, FZJ, Jülich

Brief summary of the project A standardized framework for the use of numerical linear algebra libraries on massive parallel platforms is essential for progressing application areas within supercomputing. Specifically for materials science (MS), such a framework would be pivotal in hastening the discovery and creation of new materials with beneficial properties. In this task, we will create and implement an abstraction interface that serves as an intermediary layer between the linear algebra libraries incorporated in the framework (such as ChASE and EigenExa) and the MS simulation software (e.g., libNEGF, NTChem, Yambo, etc.). Additionally, we plan to develop a new eigensolver library targeting specifically symmetric complex generalized eigenproblems as they appear in the Yambo code.

Description of the team On the Japanese side the team is made by Toshiyuki Imamura (RIKEN R-CCS) who leads the development of the EigenExa library, Kengo Nagajima (Univ.of Tokyo) who is the deputy director of the RIKEN center for Computational Science and Takahito Nakajima (RIKEN R-CCS) who leads the development of the NTChem and NTPoly codes. On the European side the team is constituted by Edoardo Di Napoli (FZJ-JSC) who leads the development of the ChASE library, Luigi Genovese (CEA) who is the main developer of the BigDFT code and the CHESS library and Alessandro Pecchia (CNR) who is the main developer of the libNEGF library. The team is complemented by researchers from the MaX, EoCoE Centers of Excellence (CoE).

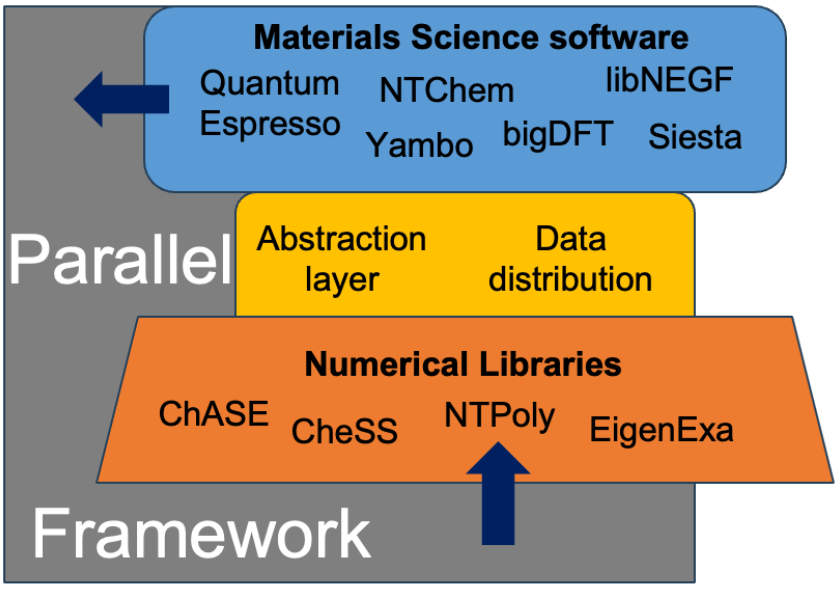

Figure 1: Schematic view of WP6.4 organization.

Recruitment and resources The FZJ-JSC partner is recruiting a postdoctoral researcher for 2 years. Such a researcher will be in charge of the main development of the Parallel Framework and will collaborate on the implementation of the generalized eigensolver to be integrated in the Yambo code. The position has been already announced and interviews are currently being carried out with a couple of

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promising candidates. We foresee to start the appointment at the latest in January 2025. Computational time projects on Japanese supercomputers have been already granted and they will be likely extended.

Collaboration strategy All the team members have already active existing collaborations which are at the base of this HANAMI task. E. Di Napoli, T. Imamura and K. Nakajima collaborate as member and main PI in two computational projects, one involving the Fugaku supercomputer (RIKEN) and one involving the Wisteria supercomputer (at University of Tokyo). A member of the T. Nakajima team (W. Dawson) is collaborating with E. Di Napoli team on the integration of numerical libraries in the ELSI interface. Luigi Genovese has a multi-year collaboration with the team of T. Nagajima. E. Di Napoli and A. Pecchia are part of the same Work Package of the EoCoE CoE. The already established collaboration is used as a starting point for the progress of the Task 6.5 HANAMI project and will be further complemented by extended on site trips to RIKEN R-CCS and University of Tokyo by the European team members during the course of 2025 and 2026 for a total of 60 days. In addition, we have discussed the possibility to exchange experiences on porting codes between FZJ-JSC and RIKEN R-CCS especially with respect to the upcoming JUPITER and Fugaku NEXT supercomputers.

Figure 2: Picture from the RIKEN-Juelich workshop (13-15 March 2024)

2.5 Task 6.5. Non-equilibrium charge-carrier dynamics in 2d-materials. Task Leader: Alessando Pecchia, CNR

Brief overview of the Task Within this task we aim at applying the bigDFT+libNEGF code, integrated in Task 6.4, to 2-dimensional heterostructures of promising materials for energy harvesting, such as TMDC type-II heterostructures (e.g., MoS/WS2 or MoS_2/WSe_2). This work is also strongly interconnected to the work carried in the EuroHPC CoE, “EoCoE-III”, where the kernel self-energies needed to simulate non-equilibrium charge carrier dynamics in these hetero-bilayers will be developed.
NTChem will provide accurate electronic properties of 2D materials, including correlations (e.g. MP2 calculations) that will be employed to validate empirical dispersion forces usually introduced in DFT calculations. This demanding calculations will be performed on the Fugaku supercomputer.
In a second phase we will explore the possibility to interface the libNEGF code to NTChem itself. This task, however, will need a careful preliminary evaluation phase due to the non-local exact exchange and the need to identify an efficient strategy for the embedding self-energy (i.e., contact self-enegies) and be subject to man power from the Japanese side. It could be, however, an occasion to develop other applications of the Green’s function formalism, such as the scattering T-matrix or CPA approaches for linear response transport in disordered systems.

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The task of interfacing BigDFT to libNEGF will be divided into 2 phases. The first task is to work at the correct ordering and indexing of the LCAO Hamiltonian matrix generated by BigDFT in order to be processable by libNEGF. A careful indexing mapping is required in order to be able to compute the embedding GFs and efficiently exploit block-dense recursive algorithms. Once this is achieved, simple non self-consistent transport calculations can be already performed.
The solution of the self-consistent Kohn-Sham equations, requires the solution of the non-equilibrium Density Matrix (libNEGF) and solution of a Poisson equation, with potential boundary conditions appropriate to transport. These software developments require a deep interaction between HANAMI scientists, at both European and Japanese sides.

Description of the team The team is composed by Alessandro Pecchia (CNR-ISMN, Rome), Edoardo Di Napoli (Juelich Supercomputing Centre, Germany), and Luigi Genovese (CEA, Grenoble) on the EU side. AP is the main developer of the libNEGF software and will perform transport calculations of hetero-bilayers of 2-dimensional materials, EDN and his team will help in porting and optimizing the code to the Fugaku architecture. LG is one of the main developers of BigDFT and will assist the interfacing with libNEGF. The Japanese side is formed by Takahito Nakajima (RIKEN Center for Computational Science) and his team, in charge of the atomistic modelling from first-principles of materials for solar energy harvesting.

Recruitment and resources A two-year postdoctoral position will be open at CNR to work at the above mentioned tasks. The selected candidate will start by end 2024 beginning 2025. Concerning the HPC resources, we have access via different projects to major European facilities, such as Juwels (FZJ), Leonardo (CINECA). libNEGF has been selected for the early access to Jupiter (exascale machine at FZJ). We plan to apply to compute time on Fugaku together with the Japanese partners on the next available calls.

Collaboration strategy The collaboration with the Japanese partners, especially with scientists at RIKEN, will initially be centered in porting the code to the Fugaku supercomputers, an effort that is likely to be non-trivial because of its Arm-based architecture. For this, the experience of the Japanese partners, already applied for instance in the developement of NTChem code, will be fundamental in order to speed up the process. In fact, the quantum chemistry code NTChem has shown very high performance on the Fugaku supercomputer. We will exchange knowledge on the strategies employed for the highly paralell DGEMM operations implemented to solve 2-electron integrals, a tensor operation that shares a lot in common with the solution to the Keldysh equation.

2.6 Task 6.6. Enhancing Materials Science scalability through innovative block sparse libraries. Task Leader: Luigi Genovese, CEA

Brief summary of the project This task will be devoted to the analysis of the scalabilty properties of the Sparse Linear Algebra manipulation operations performed in the framework of the BigDFT code. In particular, the CheSS and the NTpoly libraries will be employed and compared in terms of HPC features and convergence properties.

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This analysis will define the optimal strategy for combining the two libraries, particularly the algorithms of Fermi Operator Expansion and the Purification Method, presented in CheSS and NTpoly respectively.

Description of the team This action is lead by Luigi Genovese, maintainer of the BigDFT suite (which includes the CheSS library) in close contact with the group of T. Nakajima at RIKEN (in particular with Dr. W. Dawson, main developer of the NTPOLY library)

Recruitment and resources The project will require performance analysis of the libraries and deep interactions with the two main developers. The work will be mainly performed by CEA staff (6 PM are sufficient for the entire duration of the project) and will be carried out thanks to the lonkg-standing collaborations which exists between Genovese and Nakajima laboratories.

Collaboration strategy The collaboration is carried out on a twofold strategy. First, the main features of the two methods will be considered and investigated on a separated basis (FOE and Purification method), both in the case of scalability and of convergence properties. In particular, we expect the features to be dependent of the basis set employed for the calculation. We expect BigDFT basis sets to present optimal features for both the methods, in terms of sparsity patterns and spectrat width) Then, the combination of the two methods will be performed such as to integrate the two approaches altogether (either by the creation of a NTpoly wrapper in the CheSS library, or by the inmplementation of the FOE algorithm in NTpoly) such as to provide to the user the choice of the most optimal method for a given simulation. At the end of this task, a potential strategy to predict the most convenient method to employ for a given category of systems will be then discussed.

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3. Conclusions

All WP6 tasks have seen a very encouraging start thanks to a calibrated initial setup. As a general ground, for the majority of these tasks, the scientific activity will be built upon existing channels, already opened during previous collaborations. In the realm of WP6, HANAMI will thus have the fundamental role of consolidating these collaborations around cutting-edge problems in material science. In particular:

1. WP6.1 has posed the basis to optimize the MBPT first-principles code Yambo, specifically targeting Japanese pre-exascale supercomputers, in particular Fugaku. This collaboration will involve CNR-Nano (Modena), University of Perugia, University of Rome “Tor Vergata”, University of Tokyo, Yokohama City University, and RIKEN Center for Computational Science;
2. WP6.2 is on the way to combine the DFT code SIESTA, developed by the group at ICN2 (Barcelona), with the Effective Screening Medium (ESM) package developed by the group in Tsukuba (Japan). This task will tighten the links between ICN2 (Barcelona), CNR-Nano (Modena), the University of Tsukuba and NIMS (Tsukuba);
3. In WP6.3, two postdocs are already recruited with the aim at developing efficient workflows to allow the generation of machine learning potentials, by applying the TurboRVB QMC code to hydrogen-rich materials. This project will foster the collaboration between CNRS, Sorbonne University and NIMS (Tsukuba);
4. WP6.4 is tightening the collaboration between EU and Japan around the creation and implementation of an abstraction interface that serves as an intermediary layer between the linear algebra libraries incorporated in the framework (such as ChASE and EigenExa) and the material science simulation software (e.g., libNEGF, NTChem, Yambo, etc.). WP6.4 will be built upon collaborations involving FZJ-JSC, the CEA, the CNR, the University of Tokyo and RIKEN R-CCS;
5. WP6.5 is going to apply the bigDFT+libNEGF code to 2-dimensional heterostructures of promising materials for energy harvesting and to port the code to the Fugaku supercomputer, by exploiting the experience of the Japanese partners, already applied for instance in the development of NTChem code and fundamental in order to speed up the process. As in the case of WP6.4, this task will consolidate the links between FZJ-JSC, the CEA, the CNR from the European side with RIKEN R-CCS.
6. WP6.6 is dedicated to the merging of two HPC sparse algebra manipulation methods, in particular the Fermi Operator Expansion and the Purification Method, into a single library to be employed in the context of highly scalable HPC calculations on supercomputers. This is a relatively small task, which is going to be accomplished thanks to the mutual collaboration between the L_SIM laboratory at CEA Grenoble and the Nakajima Group at RIKEN R-CCS.

Across these projects, porting the relevant codes to the Japanese pre-exascale supercomputers is on-the-way through benchmarking or full production allocations of computational time. The financial resources allocated by HANAMI are being spent for postdoctoral contracts already signed in two cases (WP6.3) and presently running, while for most of the tasks the postdoc openings funded by HANAMI have already

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been announced and are in the candidates' selection process after their interviews. Trips to Japan by the European members to visit the Japanese collaborators are already planned and fully supported thanks to the synergy between WP3 and WP6. Beside the scientific skeleton of the ongoing collaborations, postdoc recruiting and travel funding will definitely tighten the links with the Japanese partners.

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