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Managing, simplifying and disseminating High-Throughput computational materials science with AiiDA, AiiDA lab, and the Materials Cloud Archive

The second webinar of a series presenting the most recent developments of the MaX flagship codes entitled "Managing, simplifying and disseminating High-Throughput computational materials science with AiiDA, AiiDA lab, and the Materials Cloud Archive" will be held on 27 May 2020 at 3 PM CEST.

FUNDAMENTAL RESEARCH

27 May 2020 - 27 May 2020

Online, Italy

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Description

The available computational power has steadily increased over the past decades and continues to do so, with upcoming superclusters going towards a performance on the scale of Exaflops/s. These advances present great new opportunities for computational science but also pose new challenges with respect to how to automate the resources and manage the data that will be produced.

We will give a short introduction to AiiDA, a tool that is designed to help its users leverage high-performance computing resources to automate workflows of HPC codes, such as those developed by MaX, run on those systems and manage the data that they produce. We will detail especially how the recent release AiiDA 1.0 comes with many performance improvements in the workflow engine and database in order to support high-throughput computational loads and the various mechanisms that allow its users to make

optimal use of current and future powerful HPC resources. After that, we will exhibit AiiDA lab, a GUI solution on the cloud that makes running these workflows and analyzing the results easy and intuitive, even for non-experts. Finally, we will present the renewed Archive of the Materials Cloud that serves as a dissemination platform that can be used to very easily publish data generated through AiiDA.

In this webinar, we will show how the MaX flagship code AiiDA supports its users to manage their computational workflows and the data that is produced. As opposed to all other flagship codes, AiiDA itself is not a simulation software, but instead is a workflow and data management tool. We will show how it can be used to automate workflows that directly employ the other MaX flagship codes, such as Quantum ESPRESSO, how AiiDA lab provides a user-friendly GUI to the workflows even for non-experts, and how the resulting data can easily be published through the Materials Cloud Archive.

REGISTER NOW!

Visit the official webinar page and see the exciting agenda prepared for its attendees.

MaX webinar series
This seminar is included in a series presenting the most recent developments of the MaX flagship codes. The next planned appointments are for Yambo (June 16) and CP2K (June 24). Stay tuned for the next announcements!

About MaX

MaX - Materials design at the Exascale has received funding from the European Union's Horizon 2020 under Grant Agreement n. 824143. Led by CNR (Italy), the MaX consortium partners includes SISSA (Italy), ICN2 (Spain), JUELICH (Germany), CEA (France), EPFL (Switzerland), Universiteit Gent (Belgium), CINECA (Italy), BSC (Spain), ETHZurich (Switzerland), E4 (Italy), ARM (United Kingdom), ICTP (Italy), Trust-IT (Italy).

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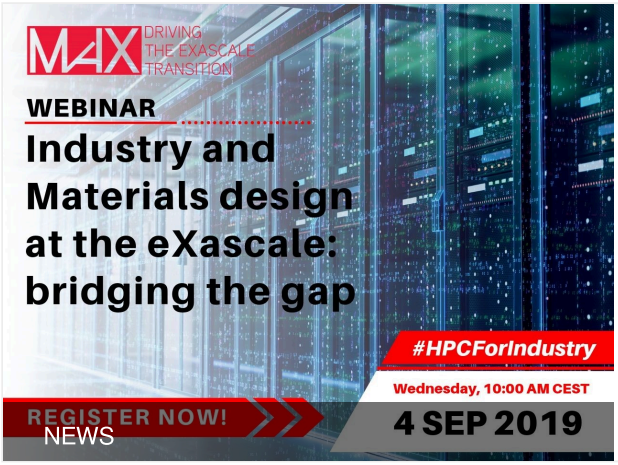

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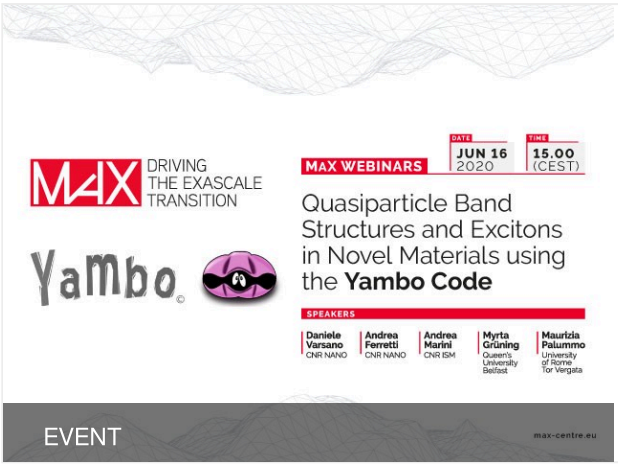

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Last update: 15 May 2020