Dr Céline Merlet wins the 2021 PRACE Ada Lovelace Award for HPC

Dr Céline Merlet
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PRACE is delighted to announce that CNRS researcher Dr Céline Merlet from the Centre Inter-universitaire de Recherche et d'Ingénierie des Matériaux (CIRIMAT) in Toulouse is the winner of the 2021 PRACE Ada Lovelace Award for HPC for her outstanding impact on HPC in Europe. Not only has Dr Merlet decisively advanced the investigation of supercapacitors with numerous innovations; she is also active in "Femmes & Sciences", an association that promotes women in science and technology. Céline Merlet will give a talk entitled "Multi-scale models and HPC for a better understanding and performance prediction of electrochemical energy storage systems" and participate in the PRACEdays21 panel discussion "Will HPC, AI, and Data Science be the same in 10 years' time?" at the EuroHPC Summit Week 2021 on Friday, 26 March 2021.

Dr Merlet's scientific track record speaks for itself: Already at the end of her PhD at PECSA laboratory (now PHENIX laboratory) in 2013, the young chemist had published a total of 10 papers in excellent international journals, 8 of which as first author. Especially her publication in Nature Materials 2012 on the molecular origin of supercapacitance in nanoporous carbon electrodes has become a key reference with more than 600 citations so far.

Back then, simulations of supercapacitors were only feasible using simplified and inaccurate electrode structures with the materials being represented by rather crude approximations like plain sheets or tubes. Dr Merlet's first key contribution to the investigation of these high-power electrochemical storage devices was to develop efficient and accurate simulations of the complex porous structures of carbon electrodes in operating systems. "This resulted in a much more realistic representation of supercapacitor's operation," Céline Merlet explains today. In fact, her results provided important insights into the device's molecular mechanisms.

Later, in her postdoc at the University of Cambridge Department of Chemistry, Dr Merlet focused on new lattice models to interpret Nuclear Magnetic Resonance experiments on supercapacitors. This required her to expand the scale of the simulations drastically to be able to calculate physical properties that are measured in experiments. In the process, Céline Merlet developed a new simulation method to examine the electrode/electrolyte interface, which is decisive for supercapacitor's efficiency. Her newly written simulation code was 10 000 times faster than previous simulation software.

Since 2017, Merlet is a CNRS researcher with her own group, and in her most recent projects, she focusses on the development of systematic multi-scale models to predict key properties of supercapacitors built of different materials, such as energy density and power density. "Through her simulations, Dr Céline Merlet has shown how HPC can help to find new classes of energy materials for a sustainable future," Prof Matej Praprotnik, Chair of the PRACE Scientific Steering Committee, points out. "Céline Merlet is a remarkable young scientist," he adds. "She develops high

performance computing methods for crucial scientific questions and is on her way to become one of the global leaders in Computational Materials Science."

As a result of her outstanding work, Céline Merlet has already won a number of scientific awards and grants, including the renowned Prix Louis Armand 2018 in chemistry, a prize awarded by the French "Académie des Sciences", or an ERC Starting Grant providing funding for 5 years to promising early career researchers.

"I am very happy that my research work has now been honoured with the PRACE Ada Lovelace Award, also because it resonates with my commitment to inspire girls and young women for science" Céline Merlet states.

She regards gender equality as a fundamental personal concern. That is why she is involved in "Femmes & Sciences", an association that promotes women in science and technology through various activities. Among else, the chemist was instrumental in the development of "Mendeleieva", a board game that encourages pupils and grown-ups to discover 125 female scientists. To promote the game and gender equality, she toured science fares and visited high school classes. "There are still too few women in scientific and technological professions and careers, and I would like to help change that by showing the kids that a successful career in science and technology is possible for both men and women", says Céline Merlet. A role model indeed.

About the PRACE Ada Lovelace Award

Launched in 2016, the PRACE Ada Lovelace Award is annually awarded to a female scientist who makes an outstanding contribution to and impact on HPC in Europe and the world, and who serves as a role model for women who are at the start of their scientific careers. The award is named after the Countess of Lovelace, a British mathematician who lived in the 19th century and among else worked with Charles Babbage on the Machine they called the Analytical Engine — one of the first precursors of computers. Many historians regard Ada Lovelace's contribution to this mechanical calculator as the very first algorithm — and herself as the first person to be rightly called a programmer.

About PRACE

The Partnership for Advanced Computing in Europe (PRACE) is an international non-profit association with its seat in Brussels. The PRACE Research Infrastructure provides a persistent world-class High-Performance Computing service for scientists and researchers from academia and industry in Europe. The computer systems and their operations accessible through PRACE are provided by five PRACE members (BSC representing Spain, CINECA representing Italy, ETH Zurich/CSCS representing Switzerland, GCS representing Germany and GENCI representing France). The Implementation Phase of PRACE receives funding from the EU's Horizon 2020 Research and Innovation Programme (2014-2020) under grant agreement 823767. For more information, see www.prace-ri.eu

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