

## **EOCOЕ: materials for energy challenge**

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EoCoE is one of the 8 centres of excellence in computing applications recently established within the Horizon 2020 programme of the European Commission. The primary objective of all the Centres of Excellence is to help strengthen Europe's leadership in HPC applications by tackling challenges in topical areas such as renewable energy, materials modelling and design, molecular and atomic modelling, climate change, Global Systems Science, bio-molecular research, and tools to improve HPC applications performance. The Energy Materials objective in EoCoE-II (2<sup>nd</sup> phase of EoCoE) will focus on three specific flagship applications in energy storage and production respectively: supercapacitor modelling, high efficiency silicon solar cells and organic/perovskite photovoltaics. Indeed advanced materials can contribute to the reduction in cost, increase in performance and extension of lifetime of the low-carbon energy technologies such as batteries, supercapacitors and solar cells. Thus, there is an urgent need for multi-functional and sustainable materials designed to provide a specific function in the final product. HPC can speed-up the entire process needed to identify new materials and to optimize them for the final use. In particular, the design of advanced materials needs to consider atomic-scale chemistry and how it affects the physical properties at larger scales till the device.