

High Performance Computing technologies to design new materials for energy applications

Massimo Celino, ENEA, C.R. Casaccia, Rome, Italy

Computational materials modelling plays a crucial role in the design of devices for efficient low cost energy generation and storage. Indeed materials modeling techniques can act as a powerful microscope to characterize the atomic-scale chemical and physical processes to design new and improved macroscopic device-scale properties. Not only high accuracy of models but also high performance computing (HPC) infrastructures, advanced ICT services and a tight collaboration among multidisciplinary experts are needed to impact deeply in the material science for energy sector at the European level. Within the recently EC promoted Centre of Excellence EoCoE (Energy oriented Centre of Excellence for computing applications, www.eocoe.eu), the potential offered by the ever-growing computing infrastructure is oriented to foster and accelerate the European transition to a reliable low carbon energy supply. Four pillars (Meteorology, Materials, Water and Fusion) are targeted in EoCoE to enhance their numerical modelling capabilities by a transversal multidisciplinary effort. A research line is fully devoted to the application-oriented design of materials at the nano-scale for more efficient devices for energy applications. New models and results in field of photovoltaics, supercapacitors and batteries will be presented.