ENEA computational infrastructure for materials design

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HPC (High Performance Computing) and BigData technologies are revolutioning how computational materials science is addressed. In a few years the new generation of supercomputers will be capable of delivering a computational power in the range of about 10^{18} floating point operations per second. The availability of this tremendous computational power opens new ways to face challenges in nanotechnology research. Materials science will be greatly affected since a new kind of dynamics between theory and experiment will be established, with the potential to accelerate materials discovery to meet the increased demand for task-specific materials. Moreover HPC will be able to analyze very large amount of data (BigData) giving access to unforeseen interpretations of both experimental and computational data. The heightened demand for automation, advanced analysis and predictive capabilities inherent to these new methods put it in an especially exciting crossroads between chemistry, mathematics and computational science. ENEA is facing these new challenges developing new methods and approaches in line with the Mission Innovation paradigm to design new materials for photovoltaics, electrochemical storage and electrolyzers.