Exploring The Next Generation Of Nanomaterials: Discovery And Materials Exploration By Multiscale Modelling At ICCRAM

S.Cuesta-López[1]

[1]International Research Center in CRMs for Advanced Industrial Technologies. University of Burgos
e-mail: scuesta@ubu.es

This is a The nature and properties of matter are the macroscopic consequence of the structure and motion of its constituent building blocks. The vision of Pierre Simon de Laplace (1749-1827), the famous French mathematician, already contained the essential ingredients and foundations of the present view of molecular dynamics. The dream of Laplace pursued the ability to predict motion by animating nature forces, providing in this way the link between the past and the future. Laplace ideas anticipate de use of force fields or forces, and appropriate numerical integration tools (analysis) to solve the motion of many-body systems like biomolecules or fluids.

A new era had started. Computers and research in molecular physics were going to evolve together across years. Physicists and mathematicians began to think in computers like tools able to analyze a system directly. Instead of merely performing a calculation, the computer became a virtual laboratory in which a system could be studied. In other words, a numerical experiment to screen and to perform materials combinatorial analysis will eventually reduce the needed to find a new product/technology and to innovate in into the market. In this context, the Genome Materials initiative was born.

Nowadays, thanks to multiscale modeling, we can design almost "a la carte" a material to fulfill the previewed operation exigencies starting from its atomic composition. This is particularly interesting in applications where experiments are difficult to perform and situations impossible to evaluate.

At ICCRAM, we are boosting the discovery of a new generation of materials with ultra-high hardness and strength, with self-healing properties against corrosion or damage, or with excellent thermodynamical properties for the storage of energy. Such a forefront technology relies on materials like nanocrystals, nanostructured metallic multilayers and metallic nano-foams. We will show examples ranging from a multiscale database initiative designed to explore new molten salts for energy applications up to new nanoscale multi-layered metallic composites (NMMCs) as systems composed by new materials with greatest radiation resistance and excellent mechanical properties.