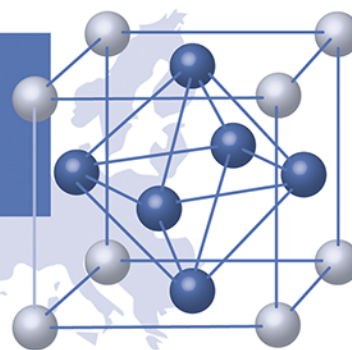


**ICCRAM Scientific Conference Series on
Advanced Materials, Critical Raw Materials
and Industrial Technologies**

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DISCOVERING NEW MATERIALS WITH THE HELP OF A COMPUTER

Dr. Sergiu Arapan

**INTERNACIONAL CENTRE IN CRITICAL RAW MATERIALS FOR
ADVANCED INDUSTRIAL TECHNOLOGIES**

**Salón de Actos de la Facultad de Ciencias
19 de Mayo de 2016
13.00 horas**

“Discovering new materials with the help of a computer”

The advance of modern computation has changed the traditional way of probing properties of matter. With the help of state-of-the-art numerical methods we can apply the fundamental laws of physics to perform virtual experiments on computers. Thus, we are witnessing the emergence of a computational materials science. Numerical simulations allow us to predict the properties of a compound based on solely the knowledge of constituting elements. Furthermore, recent implementations of statistical analysis methods and evolutionary genetic algorithms open new prospect of predicting materials with desired properties just from basic knowledge. In this presentation I'll give a short overview of some numerical techniques we are going to use within the NOVAMAG project aimed to predict new rare-earth free magnetic materials.

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