Materials Prediction By Random Searching Method

Jean-Baptiste Charraud*, Gregory Geneste, Jean-Bernard Maillet, Marc Torrent

∗ CEA, DAM, DIF F-91297 Arpajon, France
jean-baptiste.charraud@cea.fr

In a lot of domains, structure identification of new materials is a necessary step to the development of new devices with innovative functionalities. As an example one can mention the energy sector where new materials are searched to increase energy transportation and storage efficiency. To identify the most promising compounds and provide support for a precise characterization of their properties, experimental synthesis is not always enough by itself and has to be guided by numerical simulations. Algorithms using supercomputers and artificial intelligence have been introduced to predict crystal structures of new materials under specific physical conditions such as high pressure. These crystal structure prediction algorithms become a required element for the search of new promising materials. This talk is focused on a specific type of these methods called Ab Initio Random Structure Searching. Following the principles introduced by Pickard and Needs [1], it's use on supercomputers using ABINIT in conjunction with external scripts is firstly presented. This approach is driven by the search for new superconductors with possible high critical temperature that could be found in hydrogen rich alloys under pressure, called "superhydrides". It is also motivated by testing methods using Machine Learning approach. Finally the algorithm's implementation in Abinit will be discussed.

References

[1] C J Pickard, R J Needs, Journal of Physics-Condensed Matter, **23** , 053201 (2011) "Ab initio random structure searching"