Ab-initio simulations in high pressure condensed matter, fundamentals and applications

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Advances in the accuracy and efficiency of ab initio simulations and the combination of these techniques with high-pressure experiments have allowed important advances in the knowledge of the physics and chemistry of the materials under extreme conditions. These computational experiments have proven to be very efficient in high-pressure semiconductors physics [1]. In the first lecture, we will focus on the presentation of the theory involved in these studies, presenting some technical details, and also introducing some available tools. In lectures 2 and 3 we will introduce some applications of these simulations combined with high-pressure experiments showing how the study of the structural, electronic, dynamical, and mechanical properties using first-principles simulations helps in the interpretation of the experimental results and how the synergy of both techniques allow to gain insight on the physics and chemistry behind these complex experiments. The examples will focus mainly on materials with potentials applications in microelectronics, luminescence, scintillators, geophysics, etc. mainly oxides, including some orthophosphates, orthovanadates, garnets, perovskites, and other compounds that our group has studied in cooperation with other experimental groups.

[1] A Mujica, Angel Rubio, A Muñoz, RJ Needs, *Reviews of Modern Physics* 75, 863 (2003).