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Biocomputación y Física de Sistemas Complejos
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Alberto Castro Barrigón

He studied Physics at the University of Valladolid, where he completed his doctoral thesis on the modeling of materials and molecules using ab initio methods, particularly, density functional theory (DFT). Afterwards, he completed postdoctoral fellowships at the Free University of Berlin and the Fritz-Haber Institute of the Max-Planck Society. In 2009, he joined BIFI after being recruited by the ARAID Foundation of the Government of Aragon. In July 2024, he moved to the University of Valladolid, to the Department of Theoretical, Atomic, and Optical Physics.

Researcher profile

Currently, he is an R4 researcher studying the development of theoretical/computational methods for modeling materials or atomic and molecular systems. He has worked on so-called "first-principles" or "ab initio" methods, which attempt to construct modules based on the basic laws of nature, without resorting to empirical data. He is interested in the interaction between external fields and material systems, such as the prediction of the optical properties of materials or molecules by studying the interaction of light (ordinary or laser).

Importance of his research

Computational modeling is used in Physics of Materials and Chemistry, to interpret experimental data that guide future experimentation and, more frequently, to replace experiments when costs are high. This is due to improved theoretical methods, improved algorithms, and advances in computing systems. His research focuses specifically on the development of computational methodologies that enable "theoretical spectroscopy." This provides industry with the opportunity to replace expensive experimental testing with computational simulations.