Developments and applications of Materials and Molecular Sciences in within the National Center for HPC, Big Data and Quantum Computing

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The National Center for HPC, Big Data and Quantum Computing established in 2022 aims to create the national digital infrastructure for research and innovation, to form a globally attractive ecosystem based on strategic public-private partnerships for scientific and technical computing, and to promote the development of new computing technologies. It has a Hub&Spoke structure, in which a central hub coordinates and manages research programs, and ten spokes that implement the research programs in their corresponding scientific fields.
In this presentation I will describe the mission foreseen by the spoke "Materials and Molecular Sciences", focusing in particular on the discovery of new materials. The energy, environmental, and climate emergencies set the stage to a paradigm shift whereby the serendipitous discovery of natural materials is being replaced by the deliberate design of artificial ones with customised properties for specific applications. The digital revolution is the engine propelling this shift, with computers capable of processing billions of billions of information bytes per second, which make it possible to solve the fundamental equations determining the properties of complex materials in realistic device conditions and to train artificial intelligence to predict their complex emergent behaviour without even solving these equations in full detail. The Spoke involves more than 150 researchers from 12 Institutions.