



***“Complex Materials from First Principles:
From Sustainable Energy Sources to Quantum Information Science”***

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I will discuss recent progress in gaining understanding and scoping design rules for two classes of systems: *sustainable materials*, namely solids and molecules that are useful to develop sustainable energy sources, and promising *systems for quantum technologies*. I will present results obtained by carrying out first-principles simulations, coupled with computational spectroscopic techniques and, in some cases, with advanced sampling methods. I will show that, despite several approximations to the basic equations of quantum mechanics, insightful predictions on physical and chemical processes can be made that are not only corroborated by experiments, but inspire new ones. I will focus on several examples to highlight both the successes and the challenges of quantum simulations, including in the study of oxides for photoelectrodes and low power electronics, and defective semiconductors for quantum sensing applications.