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AULA ROSTAGNI

YOUTUBE STREAMING

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Complex materials from first principles: from sustainable energy sources to quantum information science

Abstract: Recent progress in gaining understanding and scoping design rules for two classes of systems will be discussed: sustainable materials, namely solids and molecules that are useful to develop sustainable energy sources, and promising systems for quantum technologies. Results will be presented, that are obtained by carrying out first-principles atomistic simulations, coupled with computational spectroscopic techniques, showing 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. Several examples will highlight both the successes as well as the challenges of quantum simulations, including the study of oxides for photoelectrodes and low power electronics, and defective semiconductors for quantum sensing applications.

Giulia Galli the Liew Family Professor of Electronic Structure and Simulations in the Pritzker School of Molecular Engineering and the Department of Chemistry at the University of Chicago, and a Senior Scientist at Argonne National Laboratory, where she is the director of the Midwest Integrated Center for Computational Materials. She is an expert in the development of theoretical and computational methods for the study of material and molecular properties using quantum simulations. She is a member of the National Academy of Sciences, the American Academy of Arts and Science, and the International Academy of Quantum Molecular Science, and a Fellow of the American Association for the Advancement of Science and of the American Physical Society.

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