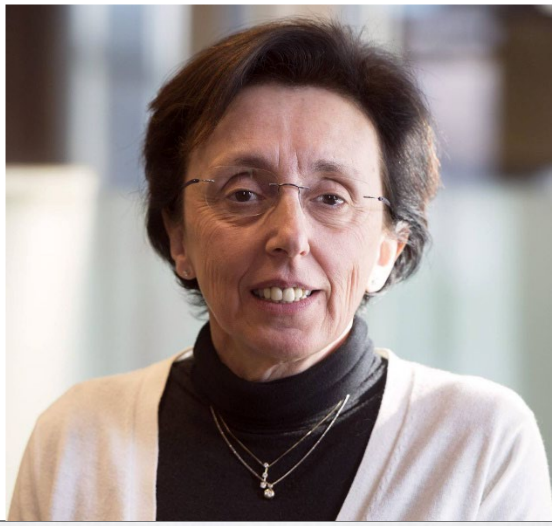
LECTURE 28



Dr. Giulia Galli

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INTRODUCTION

- Member of the US National Academy of Sciences.
- Member of the American Academy of Arts and Science.
- Member of the International Academy of Quantum Molecular Science.
- Fellow of the American Association

for the Advancement of Science and of the American Physical Society.

- Material Research Society Theory Award.
- David Adler Award and Aneesur Rahman Prize from the American Physical Society.
- Feynman Nanotechnology Prize in Theory.
- Tomassoni-Chisesi award from La Sapienza University in Italy.

Topic ：Materials for Sustainable Energy Generation and Use from Quantum Simulations

ABSTRACT

We discuss recent progress in scoping design rules for so called sustainable materials, namely solids and molecules that are useful to develop sustainable energy sources. We use simulations at the atomistic level, based on the basic laws of quantum mechanics, coupled with various methods rooted in statistical mechanics. We focus on several examples highlighting the successes and open problems of such simulations: oxides for photoelectrodes and low power electronics, and organic semiconductors for third-generation organic emitting diodes.

MINUTE

Key Topics and Concepts of the Lecture:

1. **Sustainability and Materials:**
   - **Importance of developing sustainable energy sources and clean water to mitigate environmental stress and climate change.**
   - **Historical significance of materials like silicon and lithium oxides in advancing technology and society.**

2. **Complex Materials for Energy Generation and Use:**
   - **Exploration of systems suitable for neuromorphic platforms, low power electronics, and materials for generating clean fuel from water.**
   - **Challenges in designing efficient organic light-emitting diodes (OLEDs) and membranes for removing pollutants from water.**

3. **Theoretical and Computational Strategies:**
   - **Emphasis on the need for realistic models to understand heterogeneous systems, interfaces, and defects.**
   - **Use of quantum mechanics, density functional theory (DFT), and quantum chemistry methods to study atomic and molecular behaviors.**
   - **Implementation of computational spectroscopy to validate structural models and predict material properties.**

4. **Quantum Simulations:**
   - **Importance of developing approximations and numerical methods to solve fundamental equations of quantum mechanics.**
   - **Role of artificial intelligence and machine learning in improving the efficiency of simulations.**

5. **Interdisciplinary Science:**
   - **Integration of condensed matter physics, electrochemistry, and computational methods to study light-matter interactions and solid-liquid interfaces.**
   - **Use of first-principles molecular dynamics (FPMD) and many-body perturbation theory (MBPT) for simulating and predicting material behaviors.**

6. **Materials for Sustainability:**
   - **Focus on light-activated phenomena in photoelectrochemical cells and low-power oxides.**
   - **Study of energy-efficient neuromorphic platforms and the development of theoretical and computational strategies for sustainability.**

Techniques and Methodologies:

1. **Quantum Mechanical Theories:**
   - **Density Functional Theory (DFT) for exploring phase space and molecular dynamics.**
   - **Quantum Chemistry Methods, including Hartree-Fock and hybrid functionals.**
   - **Many Body Perturbation Theory for studying light-matter interaction and computational spectroscopy.**

2. **Computational Approaches:**
   - **Use of efficient numerical methods to obtain accurate solutions and generate data for model training.**
   - **Exploration of temperature, metastability, and instabilities in phase space.**
   - **Description of interactions between matter and external fields, including light.**

Practical Applications:

1. **Designing materials for energy-efficient electronics and clean fuel generation.**
2. **Engineering membranes for water purification.**
3. **Developing materials for sustainable energy applications and addressing environmental challenges through advanced computational methods.**

The lecture emphasized the importance of interdisciplinary approaches, combining theory, computation, and practical applications to address complex problems in materials science and sustainability.