Atomic-scale modelling of organic energy materials

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In the quest for sustainable energy solutions, organic energy materials have emerged as a promising frontier, offering advantages in flexibility, cost-effectiveness, and environmental impact. This lecture will delve into the field of atomic-scale modelling, a powerful tool that provides unprecedented insights into the structure-property relationships and expedites the discovery of these materials. By employing advanced computational techniques, we can unravel the fundamental mechanisms governing the performance of organic photovoltaics, batteries, and other energy conversion and storage devices.

The lecture will begin with an overview of organic energy materials, highlighting their advantages and the challenges they face in achieving commercial viability. We will then explore the principles and methodologies of atomic-scale modelling, focusing on density functional theory (DFT) simulations. These techniques allow us to simulate and predict material behavior at the atomic level, providing a deeper understanding of electronic properties, charge transport, and stability.

Next, I will present our ongoing research on the development and applications of atomic-scale modelling tools to study the electronic structure and physicochemical processes in organic materials. The case studies will include 1) excited-state engineering of photoactive molecules with applications in solar cells, light-emitting diodes, and photocatalysis, 2) modelling of electroactive materials for redox flow batteries and polymer electrodes, and 3) development of electronic structure methods for improved accuracy of simulations.