Design of Nanoscale Materials for Energy and Environmental Applications

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Hydrogen generation and purification, carbon monoxide sequestration, solar energy conversion and energy distribution and storage are key problems that need to be resolved to achieve a sustainable energy economy and reduce, if not reverse, global warming.

In this talk I will demonstrate that key reactions involved in these processes can be achieved using specifically designed nanoscale materials. In particular, we have investigated the mechanisms of methane and water dissociation on carbon nanostructures, unraveling possible routes for a clean and sustainable H production process; we have evaluated the possibility of using carbon materials for carbon monoxide sequestration, and metal-oxide interfaces for carbon dioxide activation; we have explored ways to improve the adsorption spectra of molecular assemblies for optimal solar energy conversion; and we have studied mechanisms for optimal energy storage in polymers and nanocomposites.

All these results, based on cutting edge first principles simulations, indicate that the theoretical design of nanomaterials is an essential step for clean energy and environmental technology applications.

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