Workshop on Renewable Energy and Sustainable - WREN 2024

Toward Sustainable Innovation: Exploring the Nexus of Renewable Energies, Materials Physics, and Molecular Optics for Advanced Energy Technologies

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Abstract

The convergence between renewable energies and Materials Physics takes on an innovative dimension when considering the optical properties of molecules, focusing on the creation of efficient sensors and harnessing energy on smaller scales. In this context, electronic transport emerges as a vital link, now complemented by an understanding of optical interactions in molecules. Exploring how electrons respond to light opens a window for the design of more advanced solar cells. Specific molecules with tailored optical properties can enhance the absorption of solar energy, thereby increasing the efficiency of solar cells in converting photons into electrical current. In this context, such systems become not only energy conversion devices but also sophisticated optical sensors. By adjusting the optical properties of incorporated molecules, it is possible to create solar cells that selectively respond to different wavelengths, turning them into light-sensitive sensors. This functional duality highlights the synergy between electronic transport, optical properties, and multifunctional applications of materials. Calculations of properties such as conductivity/transmission, molecular electrical current, molecular current switching by gate field, Partial Density of States (PDOS), and hyperpolarizability are frequent calculations. These have demonstrated how molecular systems with biological interest, such as molecules found in the Amazon, or drug molecules and active principles, are studied via computational simulation with these diverse techniques, showcasing the richness of possibilities that the field of materials physics can bring. This work will present some key results from this research field, illustrating the full potential that the field of materials physics can bring to the rational and modern use of renewable energies and their application in nanodevices.

Keywords: Renewable Energies, Materials Physics, Optical Properties.