Modeling How Electric Charges Move

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Learning how to control the movement of electrons on the molecular and nanometer scales could help scientists devise small-scale circuits for many applications, including more efficient ways of storing and using solar energy. Marshall Newton, a theoretical chemist at Brookhaven Lab, presents a talk highlighting the theoretical techniques used to understand the factors affecting electron movement at the American Physical Society meeting.

"Electron transfer plays a vital role in numerous biological processes, including nerve cell communication and converting energy from food into useful forms," says Newton. "It's the initial step in photosynthesis, as well, where charges are first separated and the energy is stored for later use - which is one of the concepts behind energy production using solar cells."

Newton described how combining electronic quantum mechanical theory with computational techniques has led to a unified, compact way to understand the nature of charge transfer in complex molecular aggregates.

"In essence," he explains, "the research has led to understanding electronic transport in terms of quantitative answers to a few basic mechanistic questions: namely, how far, how efficiently, and by which route (or molecular 'pathway') a charge moves from a 'donor' to an 'acceptor' in the molecular assembly." The answers come from detailed molecular quantum calculations of the energy gaps separating the relevant electronic states, and the strength of coupling between adjacent molecular units along the "pathways."

"This new approach may yield ways to predict and control electronic transport behavior by 'tuning' the molecular components, resulting in capabilities that can be used to design new solar-based energy schemes," Newton said.

Source: Brookhaven National Laboratory