Simulation-Based Techniques Within Energy and Charge Transport of Molecular Materials: Skills and Applied Methods

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Computational methods of research are of great importance to the physical chemistry space, particularly in relation to the topic of energy and charge transport in molecular materials. Computational methods are safe, efficient, and effective ways to research potentially hazardous materials. GNU Octave is a high-level programming language with extremely useful mathematically oriented syntax utilized in energy research. The program is highly useful because of its direct applicability to simulation-based research. However, to successfully utilize Octave in the field of photovoltaics, researchers must have a good grasp of its intricacies. This project utilizes seven training exercises to successfully prepare undergraduate researchers to contribute to energy transport research using GNU Octave. Octave can be used to simulate particle interactions. Newton's kinematic equations and Euler's Method were used to create a two-dimensional dynamic system. An understanding of correct syntax, data structures, graphing capabilities, and loops was required to build this system. This simulation served as a capstone project that prepares researchers to successfully utilize Octave in the research of photovoltaic materials.