

Quantum Mechanics Derived Solutions for Sustainable Energy

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I believe that scientists and engineers have a responsibility to use our skills to improve life for all Earth's inhabitants. To this end, for the past decade I have used my skills in quantum mechanics to help accelerate discovery, understanding, and optimization of materials for sustainable energy conversion processes, from sunlight to fuels and electricity, to biodiesel combustion for transportation, to fuel cells and nuclear fusion for electricity production, to lightweight alloys for fuel-efficient vehicles. These applied investigations naturally demand the development of theoretical methods best suited to treat the phenomena or material feature of interest. Over the past three decades, my group has contributed to the development of accurate yet fast quantum-based methods for simulating molecules and materials, with the choice of techniques to develop always stimulated by an applied problem for which no suitable theoretical method exists. The cross-talk between application and algorithm is critical to the success of both. I will present selected recent examples of our methods and applications related to sustainable energy.