

# The Mueller Lecture

Thursday, November 29, 2018

4:30PM in WTHR 104

Reception 4:00PM in BRWN 4102



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## *“Theoretical Chemistry’s Role in Providing Sustainable Energy”*

### **Abstract:**

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. Concomitant with these applied investigations naturally demands 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; the choice of techniques to develop is 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. Selected recent examples of our methods and applications related to sustainable energy will be given.