Department of Chemistry Seminar

Todd J. Martinez

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"Discovering Chemistry and Photochemistry From First Principles Molecular Dynamics"

Novel computational architectures and methodologies are revolutionizing diverse areas ranging from video gaming to advertising and espionage. In this talk, I will discuss how these tools and ideas can be exploited in the context of theoretical and computational chemistry. I will show how the resulting advances in the efficiency of quantum chemistry can be harnessed to progress from traditional "hypothesis-driven" methods for using electronic structure and first principles molecular dynamics to a "discovery-driven" mode where the computer is tasked with discovering chemical reaction networks. We apply this reaction discovery method to methane pyrolysis, as an example where direct comparison to experimental results is possible. I show that the first principles method with no experimental input produces predictions in agreement with experiments and as good as bespoke models parameterized to experimental data. I then discuss the extension of these ideas to photochemical reactions involving electronic excited states. Finally, I describe our recent efforts to make computational chemistry tools broadly accessible for both education and research purposes.

STONY BROOK

Friday, April 18, 2025
1:30 pm, Chemistry 412
Refreshments 1:15 pm

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