CORE-CM SEMINAR
Michigan State University

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Discovering Chemistry with an Ab Initio Nanoreactor

Traditional approaches for modeling chemical reaction networks such as those involved in combustion have focused on identifying individual reactions and using theoretical approaches to explore the underlying mechanisms. Recent advances involving graphical processing units (GPUs), commodity products developed for the videogaming industry, have made it possible to consider a distinct approach wherein one attempts to discover chemical reactions and mechanisms. We provide a brief summary of these developments and then discuss the concept behind the "ab initio nanoreactor" which explores the space of possible chemical reactions and molecular species for a given stoichiometry. The nanoreactor concept is exemplified with an example to the Urey-Miller reaction network which has been previously advanced as a potential model for prebiotic chemistry. We briefly discuss some of the future directions envisioned for the development of this nanoreactor concept.

Thursday, April 28, 2016
12:00 NOON
Room 1400 – Biomedical & Physical Sciences
Professor Ben Levine - Host