

UNIVERSITY OF RHODE ISLAND
Department of Chemistry

SEMINAR

Room 105 Beupre
3:00 p.m, Monday, April 3, 2017

Prof. Maricris L. Mayes

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***"Advances and Applications of
Computational
Quantum Chemistry"***

HOST

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Advances and Applications of Computational Quantum Chemistry

Maricris L. Mayes

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Nowadays, theory and computation have become indispensable in various fields of chemical research and development due to its ability to provide important insights into the structures, properties, and reactivities of molecular and biological systems. In this talk, I will discuss recent theoretical and computational efforts which address some of the major challenges in quantum chemistry. The availability of high-performance computers and development of novel methods are critical to realize these challenges. In particular, I will describe developing highly accurate methods for open shell and excited states as well as for large systems with thousands of electrons. Two computational research applications will be presented: (1) the photodissociation dynamics of methane and (2) interactions and self-assembly of dipeptides.