

## FALL 2015 CHEMISTRY COLLOQUIA & CO-SPONSORED BY NCMN



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**3:15 Reception**  
**3:30 Seminar**  
**112 Hamilton Hall**

### **“Chemiluminescence and Chemiexcitation: the Gateway to Thermal Non-Adiabatic Chemistry”**

The understanding of the phenomena of chemiluminescence and bioluminescence has been extensively studied during the last few years. These processes are complicated and have an important non-adiabatic characteristics. The process involve bond breakage in association with both conical intersections, inter-state crossings and entropic traps. In this presentation I will try to give the bigger picture of the chemiluminescent and bioluminescent reaction based on our MS-CASPT2/CASSCF and ab initio molecular dynamics studies of 1,2-dioxetane, 1,2-dioxetanone, 1,2-thiazole-1,2-dioxetanone. This, in combination with studies of the firefly luciferin molecule, explains the common principles and reaction pathways of chemiluminescence and bioluminescence as well as their fundamental differences. Recent computational studies of the Dewar dioxetane reveal that additional non-radiative processes are possible. The later is an example of “dark” photochemistry as initiated with chemiexcitations. I hope that the presentation will initiate interest from other computational chemists to enter the field as well as provide method developer incentives to refine our tools with respect to accurate modelling of non-adiabatic processes on large molecular systems.

