

Science with Bob

Kieron Burke

UC Irvine

This talk is in honor of my good friend and occasional collaborator, Bob Cave. I will discuss the work we did together, when I was an assistant professor at Rutgers and Bob was visiting on sabbatical. That work was in the general area of time-dependent density functional theory in which, in collaboration with Neepa Maitra, we figured out how the kernel in linear-response TDDFT must behave in order to produce double excitations.

I will also give some updates on recent work in DFT for excitations and in other areas.

A dressed TDDFT treatment of the 21Ag states of butadiene and hexatriene Robert J. Cave, Fan Zhang, Neepa T. Maitra and Kieron Burke, *Chemical Physics Letters* **389**, 39 - 42 (2004)

Double excitations within time-dependent density functional theory linear response Neepa T. Maitra, Fan Zhang, Robert J. Cave and Kieron Burke, *J. Chem. Phys.* **120**, 5932-5937 (2004).

Theoretical Investigation of the Ground and Excited States of Coumarin 151 and Coumarin 120 Robert J. Cave, Kieron Burke and Castner, Edward W., *The Journal of Physical Chemistry A* **106**, 9294-9305 (2002)