MDPH480/PHYS480/ASTR480/MAPH480 Research Projects 2009

Project Title: Modelling of excited state absorption and femtosecond dynamics of lanthanide phosphors

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Abstract of the Proposed Research (use this page only)

The aim of this project is to model excited states of lanthanide phosphor materials as part of an on-going investigation of how to use synchrotron and femtosecond laser experiments to better understand these materials. The computational techniques that will be developed in this project will be used to design future experiments.

Concern about energy resources has motivated research seeking improved efficiency of lighting such as fluorescent tubes and white-light LEDs. Currently these high-energy states are poorly understood because conventional Ground State Absorption (GSA) reveals predominately broad features because for transitions from the ground state a 4f electron is excited into to a 5d orbital. The consequent change in bonding “shakes up” the neighbouring atoms, exciting vibrations that obscure details of the electron states.

Rather than starting with the ground state it is possible to use Excited State Absorption (ESA) by using two lasers, which one populating an intermediate step on the way up to the high-energy levels. By selecting transitions so that the second step does not “shake” the crystal it should be possible to reveal hundreds of sharp spectral lines instead the few broad bands visible in GSA experiments. It is also possible to study the dynamics of the excited states using femtosecond laser pulses, providing “snapshots” of the evolution of the electronic and vibrational states.

We have well-developed models that have been used to analyse GSA experiments. In this project we will extend those models to treat ESA and to predict the sort of signals that could be expected from experiments with femtosecond laser pulses, where there will be quantum-mechanical interference between electronic states and vibrations. This will require the student to develop a good understanding of both the computation models for the electronic and vibrational states and the theory behind advanced laser experiments.