# Computational Modelling of Cu2O at Durham University

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I will cover the recent theoretical modelling projects going at Durham University. I will talk about both modelling of ultrastrong driving of Rydberg excitons in Cu2O by a microwave field, and the simulation of simple native defects in Cu2O using density functional theory (DFT).

Firstly, the large widths of excitonic states in Cu2O allow for quasi-resonant driving of many transitions with a single microwave field. In our previous work [1,2] we have modelled this with a perturbative model for weak microwave fields. The model I will present extends agreement over a 16x increase in field strength, using Floquet theory to go beyond the rotating wave approximation into ultrastrong driving. Last year I showed the model's prediction of the absorption spectrum, and in this talk I will show the quantitative agreement we achieve in predicting the generation of sidebands on the probe laser.

In the second part of the talk I will present the simulation of all the simple native defects in Cu2O using density functional theory (DFT). Photoluminescence spectra on synthetic and natural samples reveal emission peaks deep within the band gap of cuprite [3], but the assignment of these peaks to specific defects lies on outdated theoretical work. I will cover the history of these assignments and of attempts to ground them in DFT [4]. I will compare my calculated band structures around defect sites to literature and discuss challenges with interpreting results from DFT. Chiefly, I find that in Cu2O in particular the results of calculations like these are very sensitive to the choice of approximations used, but that defects states in the band gap coming from oxygen interstitials are robust to these choices.

**References**

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