**TYC Postgraduate Student Day Abstract Submission**



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**Date of initial PhD registration:** 01/09/2015

**[Final year students only] Date of PhD submission:** 01/09/2019 **[actual/expected]**

**Which of the following presentations would you like to give:**

**Oral presentation [final year students only]** ✓(tick)  
**Poster** x (cross)

**I am interested in chairing one of the oral presentation sessions (guidance will be provided):**

**Yes** ✓(tick)  
**No** x (cross)

**Title:** Distortions and Defects in hybrid halide perovskites

**Abstract/description of your research (max 300 words):**

I use density functional theory to calculate the electronic and vibrational properties of thin-film photovoltaic materials. The majority of my PhD research has focused on hybrid halide perovskites. These materials are markedly different from their predecessors in photovoltaics – both organic and inorganic (e.g. CdTe, GaAs) – and present a number of simulation challenges [1].

Although the carrier concentration in a hybrid halide perovskite under one sun does not exceed 1016cm3, it can reach densities of 1019 cm3 under laser excitation for photoluminescence (PL) studies. I will use Effective Mass Theory to quantify the extent of electronic band non-parabolicity in CH3NH3PbI3 (MAPI). I will show that band non-parabolicity has a significant impact upon the optical effective mass, Burstein-Moss band gap shift and carrier mobility in the high carrier density regime [2]. I will also show that the slow thermalisation of above bandgap carriers, observed in PL studies, can be explained by using a classical heat diffusion model to calculate the rate of polaron cooling [3].

In the second half of my talk I will consider an imperfect crystal structure where the translational symmetry has been broken with a point defect. I will outline the lattice distortion and electronic localisation incurred when a H-centre (iodine split-interstitial with self-trapped hole) is formed in MAPI [4]. I will present on-going work related to identifying the vibrational states of this defect.

[1] J. Chem. Phys. **146**, 220901 (2017)

[2] [under review] arXiv: 1811.02281

[3] ACS Energy Lett*.*,**2** (12), 2647–2652 (2017)

[4] ACS Energy Lett*.*, **2**(12), 2713–2714 (2017)