Bartomeu MONSERRAT SANCHEZ
Theory of Condensed Matter
Cavendish Laboratory
University of Cambridge
J J Thomson Avenue
Cambridge CB3 0HE, U.K.

Optoelectronic properties at finite temperature

Abstract:

The optoelectronic properties of materials underlie a plethora of technological applications including solar cells, light emitting diodes, and flat pannel displays. Optimising the performance of these devices requires a detailed understanding of the microscopic quantum mechanical processes regulating light absorption and emission in semiconducting materials. Furthermore, as these devices need to optimally operate around room temperature, their microscopic description using first principles methods would benefit from the inclusion of finite temperature effects.

In this talk I will describe our approach to include the effects of temperature in the study of optoelectronic properties of semiconductors, including both thermal expansion and electron-phonon interactions. Our approach is based on finite difference methods, exploiting mathematical tricks such as the mean value theorem for integrals to accelerate the calculations [1,2]. I will describe the finite temperature properties of band alignments between semiconductors [3], optical absorption across both indirect [4] and dipole forbidden gaps [5], and luminescence driven by exciton-phonon coupling [6].

[1] PRB 92, 184301 (2015)
[2] PRB 93, 014302 (2016)
[3] APL 112, 193903 (2018)
[4] PRB 97, 104301 (2018)
[5] PRB 98, 161203(R) (2018)
[6] arXiv:1807.11797