Department of Physics
Condensed Matter Physics
Clarendon Laboratory, Parks Road, Oxford OX1 3PU

UNIVERSITY OF OXFORD

CONDENSED MATTER SEMINAR

Thursday 13 June at 2.15pm

"Computational Modeling and Design of Novel Perovskite Semiconductors"

Prof Marina R. Filip
Department of Physics, University of California Berkeley

Perovskites are a family of materials of unparalleled chemical and structural diversity that underpin a tremendous range of functionalities [1]. Their versatility often pushes the boundaries of chemical intuition, poses challenges for understanding their optoelectronic and structural properties, but also promises immense opportunity for materials discovery and methodological advancement. In this talk, I will presents how insight from first principles computational modeling studies of complex organic-inorganic halide perovskites has led not only to the design and discovery new perovskite semiconductors, but has also been driving the development of improved theoretical frameworks for calculating materials properties with high precision.

In the first part of my talk I will focus on the first principles computational modeling of the optoelectronic properties of organic-inorganic halide perovskites. I will first present computational modeling studies of lead-halide perovskites obtained from standard density functional theory (DFT) [2], and discuss some of the fundamental limitations of this method in the context of optical properties [3]. Next, I will give a brief introduction into the state-of-the-art methodologies beyond DFT, such as the GW approximation and the Bethe-Salpeter equation (BSE). I will present calculations of the quasiparticle band structure, band gap and charge carrier e ective masses of lead-halide perovskites [4-7], and show that the GW approach is essential in the accurate description of the optoelectronic properties of these semiconductors. Furthermore, I will present on recent advancements in understanding excitonic properties of lead-halide perovskites from first principles computational modeling within the BSE method [8], and show how this framework can be extended to study the photophysics of layered organic-inorganic perovskites.

In the second part of my talk, I will present recent work on the computational design of novel perovskites. Here I will show how the chemical landscape of perovskites can be mapped using a simple rigid-sphere geometric model [1]. I will show that this model is capable of distinguishing between perovskites and non-perovskites with a success rate of 80%, and can be used to predict large datasets of perovskites that have not been discovered yet. Finally, I will present on the computational design of a novel family of pnictogen-noble metal halide double perovskites, Cs2BB0X6, B = Bi, Sb and B0 = Cu, Ag, Au, as promising candidates for lead-free perovskite absorbers [9,10]. I will discuss theoretical and experimental work on understanding the optoelectronic properties of this class of compounds [9], as well as predictions and validations of their thermodynamic stability [11].

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Host: Prof Robert Taylor

Simpkins Lee Room, Beecroft Building