POLIMA
Center for Polariton-driven Light-Matter Interactions

SDU
Mads Clausen Institute

PROJECT TITLE

Materials discovery for low-cost and energy efficient transparent solar cells.

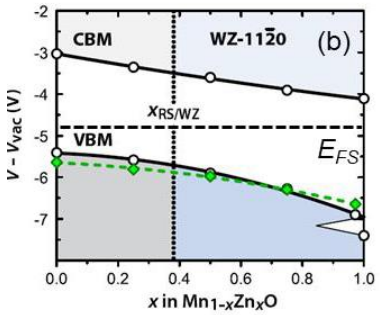
Proposed by: Line Jelver

Possible supervisor(s): Line Jelver

PROJECT DESCRIPTION

The green transition requires a significant increase in renewable energy, with solar power as the leading technology since sunlight is the largest energy source on Earth. Traditional silicon solar cells face limitations due to their rigidity, weight, and lack of transparency, restricting integration options. New organic and oxide-based thin-film solar cells, however, are flexible, lightweight, and semi-transparent, allowing for broader applications and could one day be integrated into windows and greenhouses. They also have a lower carbon footprint during production than silicon cells. Such a device can be built as a tandem system where the metal oxide front cell, will absorb near-UV light to boost overall efficiency. This placed restrictions on the metal oxides of interest as the band gap should be within the range of 2-2.5 eV to match the wavelength of UV radiation.

Illustration created by DALL-E



Bandgap variation of MnZnO alloy. From [1].

In this project, you will be trained in applying density functional theory (DFT) to enable quantum mechanical simulations of materials properties, specifically band gap predictions. The goal will be to tune the composition of a metal oxide alloy such that the band gap lies within the range of interest. The project is purely theoretical and will require that you familiarize yourself with the software performing the DFT simulations. The project will therefore consist both of a self-study part to understand the DFT method, and a practical part learning to perform and analyze the numerical calculations.

The project is part of a collaboration with the low-cost and energy efficient transparent solar cells Low cost, efficient and stable metal oxides for transparent solar cells (LESOT) research project funded by DFF which is working on the development and fabrication of such transparent solar cells and is carried out at the SDU campus in Sønderborg. As part of the project, it will be possible to visit the labs in Sønderborg and compare the calculations to experimental measurements.

[1] Haowei Peng, Paul F. Ndione, David S. Ginley, Andriy Zakutayev, and Stephan Lany, Phys. Rev. X 5, 021016 (2015)

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