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Computational Modelling using high performance computing for materials prediction and design

Thursday, 1 December 2022 14:15 (30 minutes)

The broad overarching aim is to discover novel materials suitable for high-capacity energy conversion using density functional theory (DFT) calculations and computational screening techniques. In this presentation, the application of high-performance computing facility on different materials related project is discussed as well as how this has enabled materials design and prediction. Various projects engaged in using the high-performance facility as provided by the centre for high performance computing in South Africa (CHPC) will be discussed. Firstly, 2D materials and heterostructures as possible photocatalytic materials as well as photovoltaic materials is discussed. We found that certain materials resulted in improved photocatalytic and photovoltaic properties. The reduction of platinum group metal towards the catalytic dehydrogenation of liquid organic hydrogen carriers (LOHC) is important. Pt based Sn/Co alloys were explored and found to have better dehydrogenation catalytic properties compared with pristine Pt metals resulting in cost reduction attributed with reduced Pt loading. The evaluation of doped IrO₂ for OER showed that improved catalytic properties can be obtained.

Primary author: OBODO, Kingsley (University of South Africa)

Presenter: OBODO, Kingsley (University of South Africa)

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