

Contribution ID: 220 Type: Oral Presentation

## Computational study of electronic and optical properties of graphene/brookite (210) composite

Thursday, 29 July 2021 12:45 (15 minutes)

Recently, carbonaceous nanomaterials such as carbon nanotubes and two-dimensional graphene have attracted the attention of the scientific community in probe to improve energy conversion and storage technologies. The graphene sheet is more preferred due to its large specific area, flexible structure, high transparency, excellent mobility of charge carriers and is expected to be able to slow the charge recombination. Graphene/Transition metal oxides nanocomposite study has become much of a wide interest recently with metal oxides like TiO2 and ZnO. These metal oxides are used as thin films in photovoltaic technology to harness energy. The final composite embodies both the transport properties of the former and the semiconducting properties of the latter species. This work describes an analysis of the electronic and optical properties of graphene/TiO2 studied using the Density Functional Theory (DFT) in application to dye-sensitized solar cells (DSSCs).

## Apply to be considered for a student; award (Yes / No)?

Yes

Level for award; (Hons, MSc, PhD, N/A)?

PhD

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**Session Classification:** Applied Physics

**Track Classification:** Track F - Applied Physics