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Computational studies of optoelectronic properties of CH3NH3PbI3 as a photolayer in perovskite solar cell

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Structural, electronic, mechanical and optical properties of pseudo-cubic CH3NH3PbI3 were investigated using density functional theory. The predicted values of the stated properties agreed reasonably well with the existing theoretical and experimental data. Optical studies were undertaken so as to probe the photo-physical properties of the material in order to gauge its suitability as the absorber layer in solar cell based on many body pertubation theory by solving the Bethe-Salpeter equations. Optical descriptors such as the reflectivity, refractive index, absorption coefficient and energy loss as functions of photon energy were extracted from the numerical data of the real and imaginary part of the dielectric function as per the Krammer-Kronig relations.

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

No

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

N/A

Primary authors: RUGUT, Elkana (University of Venda.); MALUTA, Nnditshedzeni Eric (University of Venda); Prof. MAPHANGA, Rapela (Council for Scientific and Industrial Research); Dr MAPASHA, Edwin (university of pretoria); Dr KIRUI, Joseph (university of venda)

Presenter: RUGUT, Elkana (University of Venda.)

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