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Solar cell performance of AgInS₂ materials from DFT and GW/BSE calculations

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Abstract content
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Ternary compounds chalcogenides are among the potential semiconductor materials for solar photovoltaic cell applications. We present first principle calculations of the electronic and the optical properties of the chalcopyrite and orthorhombic phase of AgInS₂ , using the GW many body perturbation theory built on top of the hybrid functional HSE06 orbitals. For an accurate description of the absorption spectra, we account for the quasihole-quasielectron interaction by solving the Bethe Selpeter equation (BSE). Based on the bandgaps and absorption coefficient from these calculations, we predicted the solar cell efficiency of these compounds. It is found that these compounds have GW bandgaps in the range of the experimental values and their solar cell efficiency is estimated at more than 20%.

Primary author: Dr DONGHO NGUIMDO, G.M. (University of the Witwatersrand)

Co-author: Prof. JOUBERT, Daniel (University of the Witwatersrand)

Presenter: Dr DONGHO NGUIMDO, G.M. (University of the Witwatersrand)

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