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Exciton energies of chalcopyrites AgAlX2 (X=S,Se,Te) from GW and BSE calculations

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Abstract content
   (Max 300 words)
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Using state-of-the-art Density Functional and Many Body Perturbation Theories, we study electronic and optical properties of the chalcopyrites AgAlX 2 (X=S,Se,Te). The Kohn-Sham Density Functional Theory (DFT) underestimates the fundamental and the optical gaps as a result of the
particle number dependant discontinuity in the exchange-correlation potential. Accurate estimates of fundamental gaps were obtained using post DFT Many Body Perturbation Theory at the GW level. Optical absorption spectra and optical gaps were determined from solutions of the Bethe- Selpeter Equation (BSE) in the Tamm-Damcoff approximation. Comparison of the BSE and the GW results were used to obtain exciton energies. The GW-level calculated bandgaps are in good agreement with experimental values. Exciton energies were estimated for the first time but we couldn't find any theoretical or experimental results for comparison .

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Level for award
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PhD

Main supervisor (name and email)
and his / her institution

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