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Electronic and Optical Properties of monolayer MX 2 M= Zr, Hf; X= S, Se from first principles calculations

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Abstract content
   (Max 300 words)
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Transition metal di-chalcogenide (TMDC) monolayer have potential applications in electronic and optical devices. Work on these atomically thin semiconductors is an exciting emerging field of research. In this research the electronic, photo-emission and photo-absorption properties of monolayer ZrS 2 , ZrSe 2 , HfS 2 and HfSe 2 have been investigated using density functional theory (DFT) and many body perturbation theory at the level of the partially self consistent GW 0 approximation. Solution of the Bethe-Salpeter equation (BSE) in the Tamm-Dancoff approximation was used to investigate the optical properties of these monolayer TMDCs. The structures were found to be semiconductor with band gaps within the visible range of the spectrum. Exciton binding energies were estimated from a comparison of the GW and BSE results.

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Main supervisor (name and email)
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