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2D Materials for Photovoltaic Energy Harvesting

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Abstract

Two-dimensional (2D) semiconducting materials as active layers in photovoltaic devices is a subject that has attracted a lot of attention in the last years [1]. Nowadays, the most employed materials for this kind of application are transition metal dichalcogenides (TMDCs), which are semiconductors with chemical configuration MX2 [2], where M is a transition metal such as Mo, W, and X is a chalcogen atom such as S, Se, or Te. However, many other 2D materials have also been proposed.

As far as TMDCs are concerned, while significant attention has been given to single layer TMDCs, a limited number of works have addressed the few layer case which is particularly relevant for photovoltaic devices. Herein, we studied the electronic and optical properties of few layer TMDCs composed of Mo, W, S, and Se within the G0W0 and Bethe-Salpeter approach. First-principles calculations based on density functional theory were carried out using the Quantum ESPRESSO package [3]. The many-body perturbation theory and Bethe-Salpeter calculations were performed using YAMBO code [4]. We address the photovoltaic performance of these TMDCs estimating the spectroscopic limited maximal efficiency (SLME) [5] as a function of the thickness of the semiconductor. We compared the different TMDCs to known materials used in photovoltaics paving the way for efficient nanoscopically thin solar cells.

We have also employed the same methodology described above to study a polymorph of h-BN that has been theoretically proposed recently [6]. This material, named as orthorhombic diboron dinitride (o-B2N2), is a direct band gap semiconductor. We show that the band gap energy of o-B 2N2 varies strongly with number of layers and consequently it has potential to be employed in photovoltaic devices.

References

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