Thin films of transition Metal Dichalcogenides for optical applications: a GW+BSE approach

Alexandre Reily Rocha[1]
Enérsio Marinho Júnior,[1] Cesar Perez Villegas,[2] Pedro Venezuela[3]
1. Instituto de Física Teórica, São Paulo State University (UNESP), São Paulo, Brazil
2. Departamento de Ciencias, Universidad Privada del Norte, Lima 15434, Peru
3. Departamento de Física, Universidade Federal Fluminense, Niterói, Brazil
alexandre.reily@unesp.br

Transition metal dichalcogenides (TMDCs) are semiconductors with chemical configuration MX_2 [1], where M is a transition metal such as Mo, W, and X is a chalcogen atom such as S, Se, or Te. TMDCs constitute a class of layered materials of significant interest for optoelectronics due to their scalability and thickness-dependent electrical and optical properties. While significant attention has been given to single layer TMDCs, a limited number of works have addressed the few layer case.
Herein, we studied the electronic and optical properties of few layer TMDCs composed of Mo, W, S, and Se within the G_0W_0 and Bethe-Salpeter approach. First-principles calculations based on density functional theory were carried out using the Quantum ESPRESSO package [2]. The many-body perturbation theory and Bethe-Salpeter calculations were performed using YAMBO code [3,4]. We address the photovoltaic performance of these TMDCs estimating the spectroscopic limited practical efficiency (SLME) 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.

References

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