Two-Dimensional Transition Metal Di-Chalcogenides (TMDCs) for Photovoltaic Applications

Atomically thin 2D layered semiconductor materials such as Transition Metal Di-Chalcogenides (TMDCs) have great potential for use as flexible, ultra-thin photovoltaic materials in solar cells due to their favorable photon absorption and electronic transport properties. The electronic properties, such as band structure and bandgap, and optical absorption properties of Tungsten Disulfide (WS_2) were obtained from Density Functional Theory (DFT) calculations; the properties of WS_2 make it a favorable photovoltaic material. Using these properties, a solar cell based on monolayer and bulk WS_2 together with amorphous silicon (a-Si) was modeled using numerical calculations and simulations. The maximum efficiency of this cell is 23.3% with V_{OC} 0.84 V and J_{SC} 33.5 mA/cm^2. The performance of this solar cell is comparable to many commercial cells. The results show that WS_2 can serve as a suitable photovoltaic material, opening possibilities to develop solar cells based on 2D TMDCs. As conventional photovoltaics approach the Shockley-Queisser limit, the need for unconventional materials and approaches has become more apparent. Hybrid alloys of TMDCs exhibit tunable direct bandgaps and significant dipole moments. Dark state protection induced by dipole-dipole interactions forms new bright and dark states in the conduction band that reduce radiative recombination and enhance photon-to-electron conversion, leading to significantly higher photocurrents. In my work, current enhancement of up to 35% has been demonstrated by modeling dark state protection in a solar cell composed of Tungsten Diselenide (WSe_2) and Tungsten Sulfo-Selenide (WSeS) with an ideal maximum efficiency exceeding the Shockley-Queisser limit.