

Proposal of a dual-gated WTe₂/MoSe₂ van der Waals tandem solar cell

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We propose and numerically investigate a tandem solar cell (Fig. 1) based on van der Waals heterostructure [1] composed of two monolayers of transition metal dichalcogenides. The electronic connection between the two subcells is obtained *via* tunneling through the heterojunction, electrostatically controlled by means of a dual-gate. Tuning the dual-gate voltages also provides a way to match the photocurrents in the two subcells.

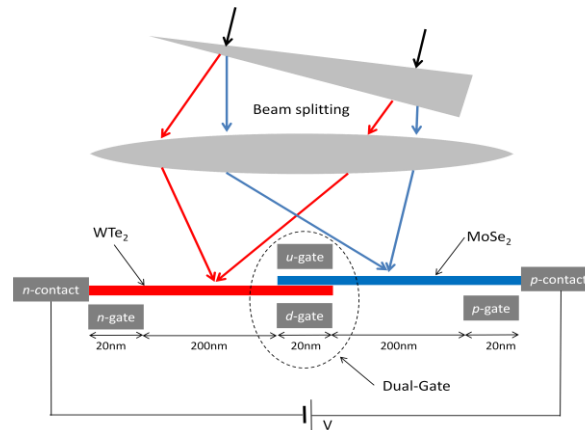


Fig 1 : Schematic representation of the tandem solar cell associated with a beam splitting system. The WTe₂ and MoSe₂ subcells are connected via a heterojunction enclosed in a dual-gate system (u- and d-gates). The cell is contacted through the electrodes denoted as n- and p-contacts, while the purpose of the n- and p-gates is to electrostatically dope the layers.

As shown Fig. 2, the tunable dual-gate allows to obtain a V_{oc} very close to the maximum achievable: 1.54V versus 1.55V for the sum of those of the two single subcells. Moreover, we observe an excellent fill factor of 0.89 compared to 0.85 and 0.89 respectively for WTe₂ and MoSe₂. By assuming an optimal absorption, as expected in light-trapping systems, we estimate that a power conversion efficiency of 30.7%, largely exceeding that of single subcells (17.5 and 23.0% respectively for WTe₂ and MoSe₂), could be attained. Although this result should be tempered by the increase of the technological challenge associated to the realization of the light trapping and beam splitting systems, it nevertheless clearly indicates that transition metal dichalcogenides monolayers can be an option for future high efficiency photovoltaic.

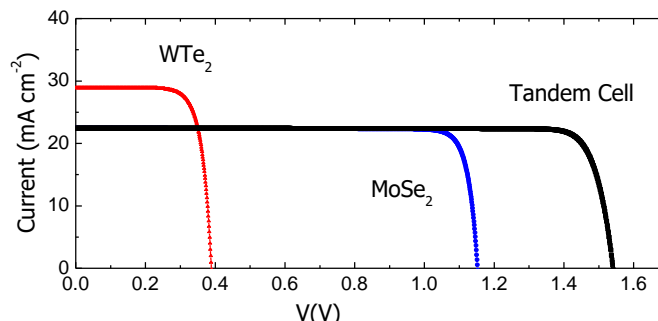


Fig 2 : Calculated current-voltage characteristics for the single subcells (WTe₂ and MoSe₂) and the tandem solar cell. Our calculation are based on ab-initio model for band diagrams [2] and derive-diffusion model for currents [3].

[1] Pospischil, A.; Furchi, M. M.; Mueller, T. Nature Nanotechnology 2014, **9**, 257–261.

[2] Szabo, A.; Koester, S. J.; Luisier, M. IEEE Electron Device Letters 2015, **36**, 514–516.

[3] Burgelman, M.; Nollet, P.; Degraeve, S. Thin Solid Films **2000**, 361-362, 527–532.