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Getting the Most from 2-D Materials: the Role of Device Dimensionality HUASHAN LI, DAVID STRUBBE, JEFFREY GROSSMAN, Department of Materials Science and Engineering, Massachusetts Institute of Technology — While the control of material dimensionality has been widely used as an important design means, the device dimensionality, which relates to the regularity of the material ensemble rather than the material itself, has received far less attention. Recently, both vertical [1,2] and lateral [2] heterojunctions based on 2-D materials have been successfully synthesized, which provides an unprecedented opportunity to renew our understanding of the concept of "dimensionality." In this study, we propose a design strategy of controlling device dimensionality by computationally investigating a "1.5-dimensional" solar cell device made of a 2-dimensional graphene based material. According to the predicted optical properties and charge dynamics, this prototype system has the potential to achieve desirable characteristics of robustness against defects, efficient polaron pair dissociation, broad tunability with surface functionalization and the possibility to form tandem cells. In addition, the optimization of correlated light harvesting procedures simultaneously becomes attainable in such 1.5-d solar cell due to the extra degree of freedom to manage the flux of mass and energy.

[1] Geim, A. et al., Nature, 2013, 499, 419-425
[2] Gong, Y. et al., Nat. Mater. 2014

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