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Computational Spectroscopy for Nanoscale Photovoltaics

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Nanoscale photovoltaic (PV) systems employ nanomaterial interfaces to dissociate bound excitons formed upon sunlight absorption. This mechanism results in a correlated electron, hole, and exciton interface dynamics whose accurate determination is challenging both theoretically and experimentally. In this talk, I will discuss approaches available to compute and combine relevant spectroscopic quantities to predict efficient nanoscale PV systems. Further, I will present our recent work on two novel families of nanoscale PV devices based on: 1) Nanocarbon materials, achieving 1.3% efficiency, tunable infra-red optical absorption, and superior photostability compared to organic solar cells 2) Two-dimensional monolayer semiconductors such as Graphene-BN and MoS_2, capable of absorbing a significant fraction of sunlight within just $\approx$ 10nm, and showing tunable absorption, band offsets, and power conversion efficiency (PCE).

In closing, I will discuss the errors and necessary accuracy in predicting PCE from first-principles calculations, and propose a suitable figure of merit to quantify absorption solar-matchedness to be used in large-scale searches of nanoscale PV materials.