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Doping Metal-Chalcogenide Quantum Dot Solar Cells for Enhanced Device Performance

Abstract.

II-VI semiconductor quantum dots (QDs) have received enormous attention in recent years owing to their unique electronic and optical properties. Among II-VI semiconductors, cadmium sulfide (CdS) has a relatively large direct optical band gap of 2.42 eV, corresponding to an optical cut-off absorption at 515 nm, while zinc sulfide (ZnS) has an optical band gap of 3.54 eV and an absorption cut-off at 350 nm. Owing to the quantum confinement effect, the CdS and ZnS quantum dots have unique properties different from the bulk. These quantum dot materials are excellent candidates for applications in optoelectronics and photonics, but making these materials into competitive photovoltaics requires a reduction of the band gap, so as to absorb more sunlight, and doping both p-type and n-type permitting the construction of p-n diode structures. One way to improve the efficiency is to tailor the band-gap of the device materials. There exist many ways to tailor a material's band-gap: one example is introducing dopants, such as Mn dopants in II-VI semiconductor quantum dots. Understanding how a dopant influences the band structure is vital to better band-gap engineering and thus achieving higher efficiency photovoltaics. This team has recent results, although unpublished, that shows CdS and ZnS quantum dots can be doped both p-type (hole carriers) and n-type (electron carriers), as seen in prior metal chalcogenide work by members of this team [2]. The plan is to explore how these materials can be proficiently doped to make effective and efficient solar cell diode structures, but using chemical synthesis methods, for device fabrication. Combining this effort in doping these sulfide materials with chemical fabrication techniques provides an obvious route to large scalability, i.e. allows for mass production at low cost. The doping efforts will be guided by theory, using established expertise in density functional theory.