Mechanochemical engineering of halide perovskites and ZnO quantum dots for game-changing improvements in light harvesting devices

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Perovskite solar cells (PSCs) are the most emerging area of research among new generation photovoltaic technologies. The power conversion efficiency (PCE) of PSCs has rapidly increased since their first demonstration in 2009 from 3.8% to a current certified value over 26% thanks to continuous improvements of fabrication protocols and the underlying physics. Both the perovskite absorber layer and the electron-transporting layer (ETL) are key elemenents for improving performance of PSCs.

The preparation of metal halide perovskites (MHPs) has commonly relied on solution-based methods. While this approach is relatively versatile, it faces challenges such as limitations in their compositional engineering or long-term storage. An alternative approach is solvent-free mechanochemical synthesis by grinding the solid reactants that was pioneered by our group in 2015.[1] The lack of the solubility limitation in mechanochemical synthesis paved the way for compositional engineering of various phase-pure MHP compositions that could not be obtained by wet methods. Strikingly, PSCs fabricated from mechanoperovskites exhibit superior photovoltaic performance compared to conventional devices made using the classical wet-chemical procedure.[1]

ZnO is a very promising ETL in thin-film photovoltaics. However, the poor chemical compatibility between perovskites and commonly used sol-gel-derived ZnO nanostructures makes challenging fabrication of efficient and stable PSCs. Our group has recently developed new organometallic approaches to high-quality ZnO QDs that led to the breakthrough in the field.[2,3] For example, PSCs based on low-temperature processed ETL composed from processable organic ligand-free ZnO QDs reached the PCE of 20.05% with no need for the ZnO/perovskite interface passivation.[3], i.e., the state-of-the-art performance among reported non-passivated pure ZnO-based PSCs. In turn, ZnO QDs capped with a zwitterion afforded the device with one of the highest performances (PCE of 21.9%) reported for ZnO-based PSCs, and competitive stability.[4]

Finally, our view on current challenges and future directions in this interdisciplinary area of research will be provided.

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