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Development of New Solar Energy Conversion Materials Based on sp Hybridization Theory[1] WEICHANG HAO, Beihang University — The electron structure of the semiconductors can determine the absorption characters for solar spectrum, and it also determined the excitation, transform and recombination of the electro-hole pairs. According to the band theory of semiconductor, above physical processes always depend on the essential electronic properties such as the band gap, the position of the Fermi level, and the effective mass of the materials. Therefore, the variation of these structure properties may have great effect on the solar energy conversion process. For example, crystal, defects, surface states (include reconstruction and mismatch of the atoms), lattice distortion, and so on can modulate those electronic structure. During the recent years of researching, we gradually found that the materials with *sp* hybridization may develop appropriate electronic structure which is benefit to obtain high-efficiency materials with enhanced light absorption and mobility of the electrons and holes. The main idea is that the sp hybridization orbital is spatially anisotropic and by choosing the applicable elements will form the dispersive band in the CBM and VBM. we can obtain lower effective mass and higher mobility of the electrons and holes, and it is hopeful to find some high-performance solar energy conversion materials via this strategy. .

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