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Single Element n-p Co-doped Wide Band-gap Semiconductors as Candidate Materials for Intermediate-Band Solar Cells[1] GUANGFEN WU, CHUNLEI YANG, GUOHUA ZHONG, Shenzhen Institutes of Advanced Technology,China, XUDONG XIAO, Shenzhen Institutes of Advanced Technology,China and The Chinese Univ. of Hong Kong, Hong Kong, China, ZHENYU ZHANG, University of Science and Technology of China — Non-compensated n-p codoping by different element combinations has proven to be an effective approach to introduce intermediate bands in wide band-gap semiconductors. In this approach, the electrostatic attraction within an n-p dopant pair helps to enhance both the thermodynamic and kinetic solubilities of the dopants. Here we present a conceptually new and appealing approach to achieve non-compensated n-p codoping by substitutionally occupying the anionic and cationic sites in the host materials with a single element. The validity of this approach is demonstrated using first-principles calculations, showing that half filled energy bands are created within the forbidden gaps of the semiconductors because of the non-compensated nature of the codpants. Moreover, the electrostatic attraction between the neighboring dopant pairs enhances their thermodynamic and kinetic solubilities in the host semiconductors. Efforts on experimental confirmation of the single element n-p co-doping concept will also be discussed.

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