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**Origin of doping bottleneck in semiconductor quantum dots** SU-HUAI WEI, National Renewable Energy Lab, JINGBO LI, SHU-SHEN LI, JIAN-BAI XIA, Institute of Semiconductors, Chinese Academy of Sciences — Doping difficulties in semiconductor nanocrystals have been observed and its origin is currently under debate. It is not clear whether this phenomenon is energetic or depends on the growth kinetics. Using first-principles method, we performed systematic study of defects (donors, acceptors, isovalent defects, etc.) in ZnSe quantum dots. we show that, the transition energies and defect formation energies of the donor and acceptor defects always increase as the quantum dot sizes decrease. However, for isovalent impurities the changes of the defect formation energies are rather small. Our study suggests that for donor and acceptor defects, the doping difficulty is mostly due to energetic effects, whereas for isovalent impurities, the doping difficulty is mostly due to kinetic effects. The origin of the calculated trends is explained using simple band-energy-level models.

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