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Quantum confinement effect on Li-Segregation in Si nanowires CHUAN-DING DONG, XIN-GAO GONG, RU-QIAN WU, DEPARTMENT OF PHYSICS, FUDAN UNIVERSITY, SHANGHAI 200433, CHINA COLLABORATION, DEPARTMENT OF PHYSICS AND ASTRONOMY, UNIVERSITY OF CALIFORNIA, IRVINE COLLABORATION — Silicon nanowires (SiNWs) have attracted extensive research attention due to their excellent properties that are promising for various applications. The incorporation of impurity atoms and change of size play a crucial role in the control of their electronic properties. Using density functional calculations, we studied the segregation behavior of Li atom in SiNWs with different sizes. It is striking that the doping and segregation energetics also strongly depend on the size of SiNWs. Doping Li into the nanowire with a diameter less than 1.3 nm is energetically unfavorable. In contrast, Li prefers to take the center sites in large SiNWs. The phenomenal size dependence can be understood through the quantum confinement effect toward the electronic states introduced by the Li atom. The reduced size also leads to strong quantum confinement for states at the conduction band minimum and increases their energies. We will discuss other properties of Li in SiNWs, which are important for applications such as using SiNWs as electrode materials in Li-batteries.

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