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Strain-Enhanced Doping in Semiconductors: Effects of Dopant Size and Charge State[1] JUNYI ZHU, 1 National Renewable Energy Lab 2 University of Utah, FENG LIU, GERALD STRINGFELLOW, University of Utah, SUHUAI WEI, National Renewable Energy Lab — When a semiconductor host is doped by a foreign element, it is inevitable that a volume change will occur in the doped system. This volume change depends on both the size and charge state difference between the dopant and the host element. Unlike the "common expectation" that if the host is deformed to the same size as the dopant, then the formation energy of the dopant would reach a minimum, our first-principles calculations discovered that when an external hydrostatic strain is applied, the change of the impurity formation energy is monotonic: it decreases if the external hydrostatic strain is applied in the same direction as the volume change. This effect also exists when a biaxial strain is applied. A simple strain model is proposed to explain this unusual behavior, and we suggest that strain could be used to significantly improve the doping solubility in semiconductor systems.

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