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Why Cu diffuses fast in semiconductors? JIE MA, SU-HUAI WEI, national renewable energy lab — It is well-known that experimentally Cu diffuses fast in semiconductors and the fast diffusion plays an important role in many applications. However, the theoretical reason for the fast diffusion is still unclear. Using first-principles calculations, we compare the diffusion behavior between Cu and group-IA atoms in CdTe, and find that the fast diffusion of Cu can be explained by the existence of the symmetry-induced strong s-d coupling in the system, which lowers the energy significantly at the site usually consists the barrier for group-IA system. Due to this s-d coupling, the most stable doping site, diffusion pathway, and diffusion energy curve of Cu are different from those of group-IA atoms, and the diffusion barrier for Cu+ is usually larger than that for neutral Cu. The mechanism is expected to be general for all tetrahedral semiconductors.

Jie Ma
national renewable energy lab

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