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Origin of the distinct diffusion behaviors of Cu and Ag in covalent and ionic semiconductors SU-HUAI WEI, Beijing Computational Science Research Center, HUI-XIONG DENG, JUN-WEI LUO, SHU-SHEN LI, Institute of Semiconductors, Chinese Academy of Science — Group IB elements Cu and Ag are important contact materials in semiconductor devices due to their low resistivity. However, they have shown puzzling diffusion behaviors in semiconductors: Cu diffuses much faster than Ag in covalent semiconductors like Si and GaAs, but Ag diffuses faster than Cu in more ionic II-VI semiconductors such as CdS and CdTe despite Ag has larger size than Cu. In this work, we reveal the underlying mechanisms of these different diffusion behavior by combining the first-principles calculations and group theory analysis. We identified the important roles of the crystal symmetry enforced s-d coupling as well as the Coulomb energy and strain energy in determining the diffusion behaviors of Cu and Ag in the covalent and ionic semiconductors. We show that the s-d coupling is absent in pure covalent semiconductors but increases with the ionicity of the zinc-blende semiconductors, and the coupling strength of Cu, owing to its higher d orbital energy, is much larger than Ag. In conjunction with the Coulomb interaction and strain energy, the s-d coupling is able to explain all the diffusion behaviors of Cu and Ag in covalent to ionic semiconductors. H.-X. Deng, J.-W. Luo, S.-S. Li, S.-H. Wei, Phys. Rev. Lett. 117, 165901 (2016).

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