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Origin of the co-dopant induced enhancement of ferromagnetism in (Zn,Mn)O YAN ZHU, JUEXIAN CAO, Department of Physics and Astronomy, University of California, Irvine, California , Z.Q. YANG, Surface Physics Laboratory (National Key Laboratory), Fudan University, Shanghai 200433, China, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine, California 92697-4575, USA — Using the density functional calculations, we elucidate the mechanism of co-dopant induced enhancement of ferromagnetism of (Zn,Mn)O. Li and Cu atoms tends to segregate toward Mn atoms and strongly promote the ferromagnetic coupling via either RKKY or superexchange interaction. The hole states produced by either Li or Cu are rather delocalized and they are efficient in mediating magnetic ordering. These findings shed new light for the design of dilute magnetic semiconductors with co-dopants for spintronic applications.

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