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Predictive modeling of dopant control in semiconductors for spintronics and solar energy applications using non-compensated n-p codoping[1] W. G. ZHU, University of Tennessee & Oak Ridge National Laboratory, Z. Y. ZHANG, Oak Ridge National Laboratory & University of Tennessee — We apply a recently established non-compensated n-p codoping approach (W. G. Zhu et al, Phys. Rev. Lett. in press) for the design of oxide-based diluted magnetic semiconductors with enhanced Curie temperatures for spintronics and carbon-based two-dimensional nanostructures with appropriate band gaps for solar energy applications. Using first-principles calculations within density functional theory, we demonstrate that the magnetic dopant concentration can be greatly enhanced in ZnO with the use of this approach. The resulting magnetic property will be discussed. We also apply this approach to tune the band gap of graphene-based nanostrucures to around 2 eV for potential solar energy applications.

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