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Ferromagnetism in ZnO doped with alkaline elements YIREN WANG, JINGYUAN PIAO, GUOZHONG XIN, Univ of New South Wales, YUNHAO LU, Zhejiang University , ZHIMIN AO, University of Technology Sydeny, NINA BAO, JUN DING, National University of Singapore, SEAN LI, JIABAO YI, Univ of New South Wales — We have observed room temperature ferromagnetism (RTFM) in ZnO doped with alkaline elements Using first-principles calculations we found the magnetization in these systems is originated from the O2p hole states around Zn vacancies. Calculations indicate that the formation energy of Zn vacancies alone is rather high while further investigation indicates the formation can be much stabilized by the alkaline dopants in the form of defect complexes. By calculating the formation energy of concerned defects and complexes, we found the role of the dopants that under a certain doping concentration: Zn vacancy, substitutional and interstitial dopants can form a defect complex, which can lower formation energy, therefore stabilizing Zn vacancies. Moreover K dopants have shown unique functions on the ferromagnetism since the substitutional K can induce magnetic moments to the system by forming partial zinc vacancy via lattice distortion. Hence K doped ZnO can be magnetic at low doping concentrations. Experimentally, Li, Na doped ZnO films and K doped ZnO nanorods with different doping levels are synthesized, RTFM can be observed in all these systems. The magnetization is found to be greatly influenced by the doping concentrations. The experimental results have shown good consistence with our theoretical calculations. Our studies can inspire the defect induced ferromagnetism as a new route for the fabrication of new diluted magnetic semiconductors.

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