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Enhanced formation of Zn-interstitials by their attractive interactions with O-vacancies in ZnO[1] YONG-SUNG KIM, Korea Research Institute of Standards and Science, Daejeon, South Korea, C.H. PARK, Pusan National University, Pusan, Korea — O-deficiency is known to give n-type doping in ZnO without intentional dopants. Even though the native defects, O-vacancies and Zn-interstitials, have been excluded theoretically as the main sources of the n-type doping, experiments have still shown the close relationship between the n-type doping and the O-deficiency. In this work, we investigated the interactions between the O-vacancies and Zn-interstitials in ZnO based on density-functional theory calculations, and propose that the formation of Zn-interstitials can be significantly enhanced by the attractive interactions with O-vacancies. The enhanced formation of Zn-interstitials can be an important source of the n-type doping in O-deficient ZnO.

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