Supplementary Information for

Distribution and self-assist diffusion of Be, Mg impurities in ZnO

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1. Isosurfaces of charge density for the peaks in DOS introduced by $\beta - Be_i$, $(2Be)_{Zn}$, $(2Be)_{Zn} - Be_{Zn}$, and $(2Be)_{Zn} - Mg_{Zn}$. The positions of these peaks in DOS can be seen in Fig. 3 (a-c).

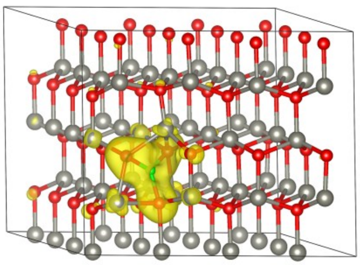

Fig S1. Isosurfaces of charge density for p0 peak in DOS for the ZnO system containing a β-Be_{Zn} defect.

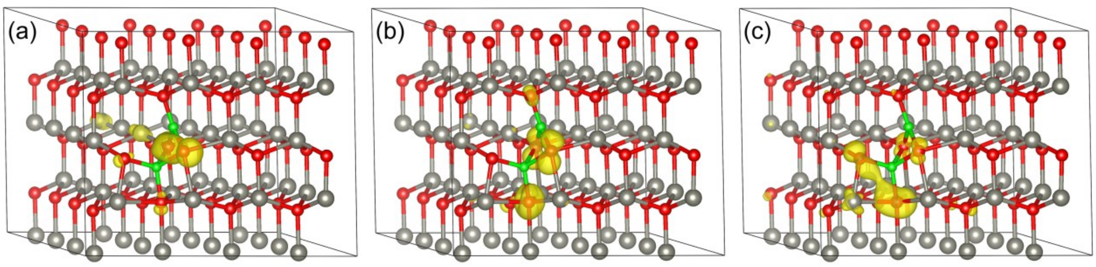

Fig S2. Isosurfaces of charge density for (a) p1, (b) p2, and (c) p3 peaks in DOS for the ZnO system containing a $(2Be)_{Zn}$ defect complex, respectively.

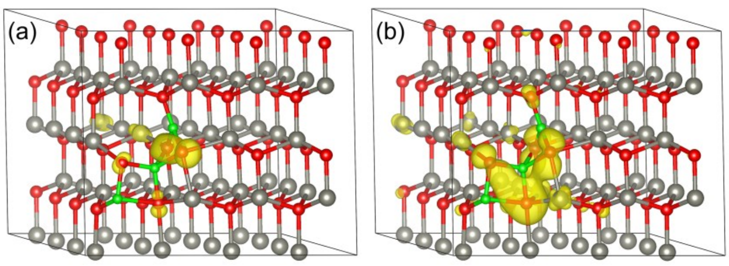

Fig S3. Isosurfaces of charge density for (a) p1 and (b) p2 peaks in DOS for the ZnO system containing a $(2Be)_{Zn} - Be_{Zn}$ defect complex, respectively.

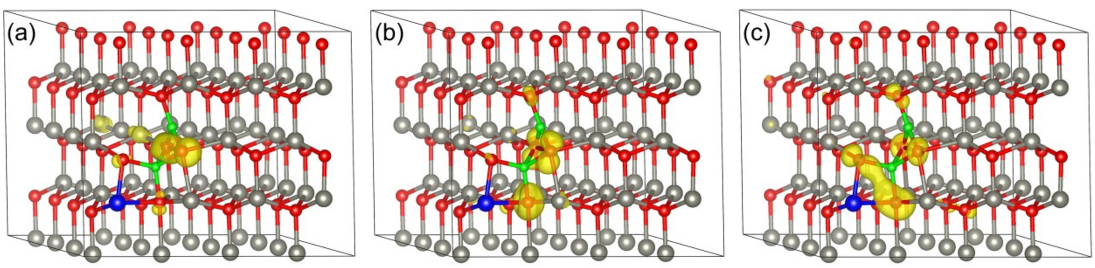

Fig S4. Isosurfaces of charge density for (a) p1, (b) p2, and (c) p3 peaks in DOS for the ZnO system containing a $(2Be)_{Zn} - Mg_{Zn}$ defect complex, respectively.

2. The diffusion feature of Be in ZnO with Mg_{Zn} defect.

Besides the Be_{Zn} defect, Mg_{Zn} defect may also influence the diffusion feature of Be. With a careful examination of the migration paths of Be as it is close to a Mg_{Zn}, we find that the influence of Mg_{Zn} defect on the diffusion feature of Be is quite weak. As shown in Fig. S5, energy barriers of all these migration paths maintain their basic feature as in pure ZnO matrix. The differences of energy barriers can be attributed to the repulsive interaction between Mg_{Zn} and Be_i, which is very local. Its diffusion behaviors could be influenced slightly as Be diffuses close to Mg_{Zn},.

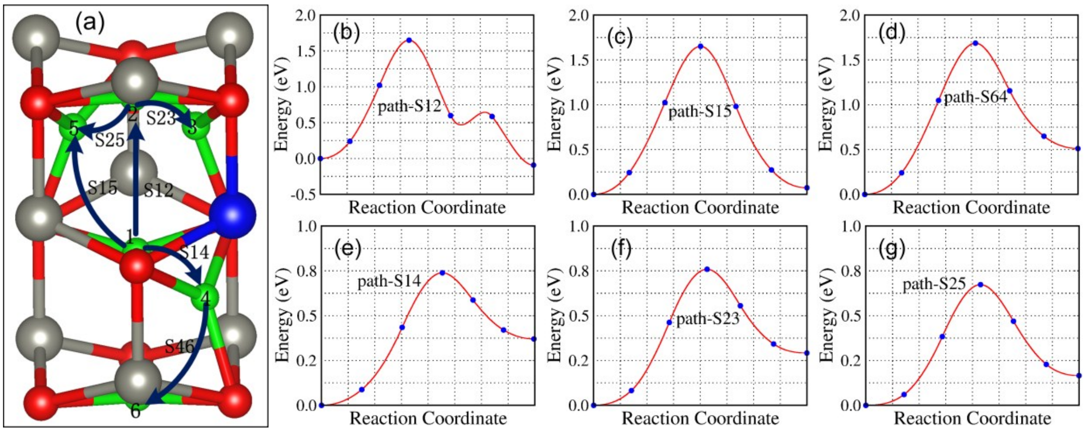

Fig S5. (a) Schematic representation of the possible diffusion paths of Be in ZnO around a Mg_{Zn}. The gray, red, blue and green balls represent Zn, O, Mg and Be atoms, respectively. (b-g) The energy barriers of corresponding migration paths that shown in (a).