Supporting Information

Influence of doping effect on zinc oxide by first principles studies

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In our paper, we perform DFT calculation to discuss the influence of doping effect on zinc oxide. Specifically, we study the influence of magnetic dopants (Mn or Co). For comparison, here we report the same DFT calculation results as in the main body of our paper, but without the consideration of spin configuration of Mn and Co. And the calculation results reveal the same conclusion. Figure S1 shows that the transition pressure decreases with Mn doping (6.25% for Figure S1a and 12.5% for Figure S1b). Figure S2 shows that the transition pressure decreases with Co doping (6.25% for Figure S2a and 12.5% for Figure S2b). Figure S3 shows that the transition barrier of ZnO decreases with Mn doping (Figure S3a) or Co doping (Figure S3b).

These calculation results indicate that magnetic dopants are not necessary for decreasing the transition pressure / barrier of ZnO.

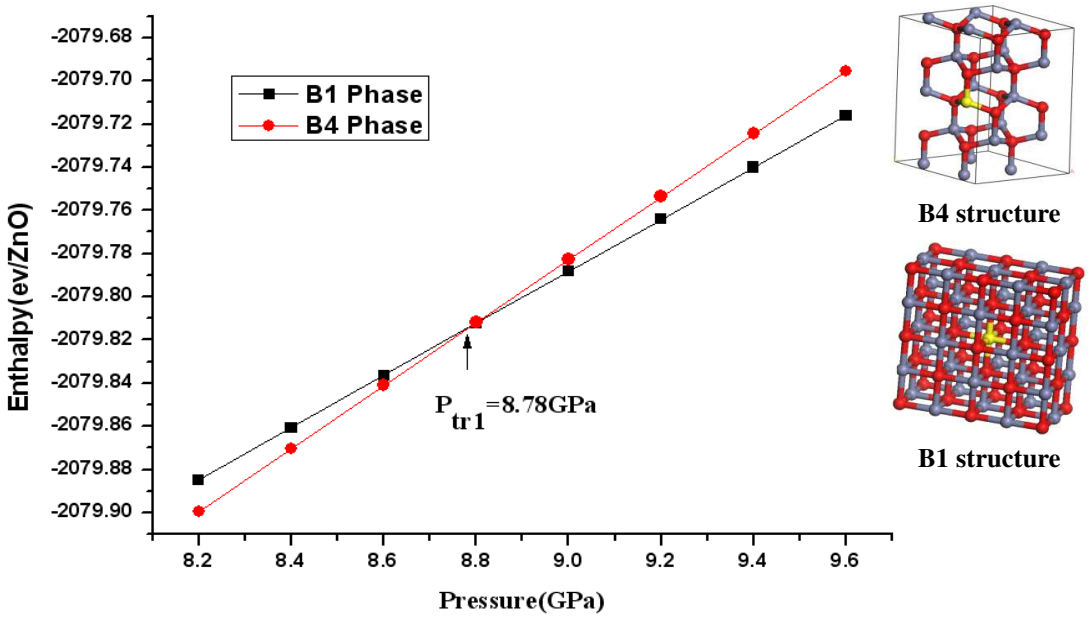

Figure S1 (a) The enthalpy as a function of pressure at temperature T=0 for B4 and B1 of Mn-doped ZnO from calculations. The simulation cell includes 32 atoms, which is equivalent to a Mn concentration of 6.25% ($Zn_{15}Mn_1O_{16}$). The picture shows more than 32 atoms in the cell since the atoms on the surface and the corner are shared by adjacent cells;

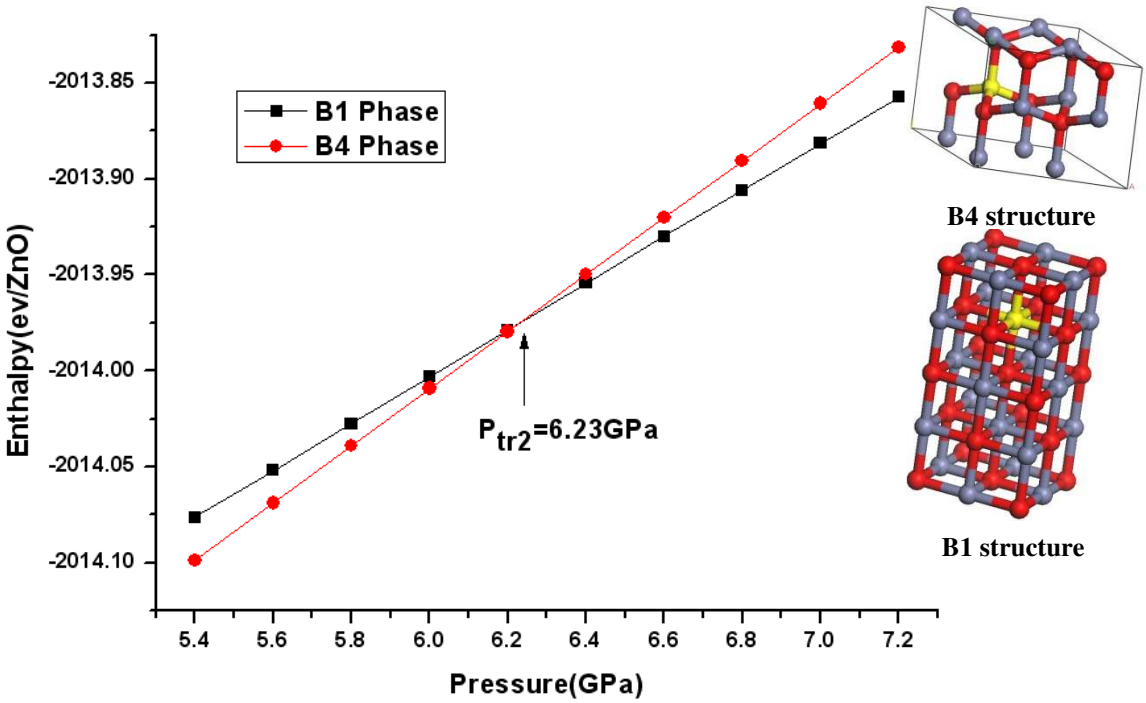

Figure S1 (b) The enthalpy as a function of pressure at temperature *T*=0 for B4 and B1 of Mn-doped ZnO from calculations. The simulation cell includes 16 atoms, which is equivalent to a Mn concentration of 12.5% ($Zn_7Mn_1O_8$). The picture shows more than 16 atoms in the cell since the atoms on the surface and the corner are shared by adjacent cells.

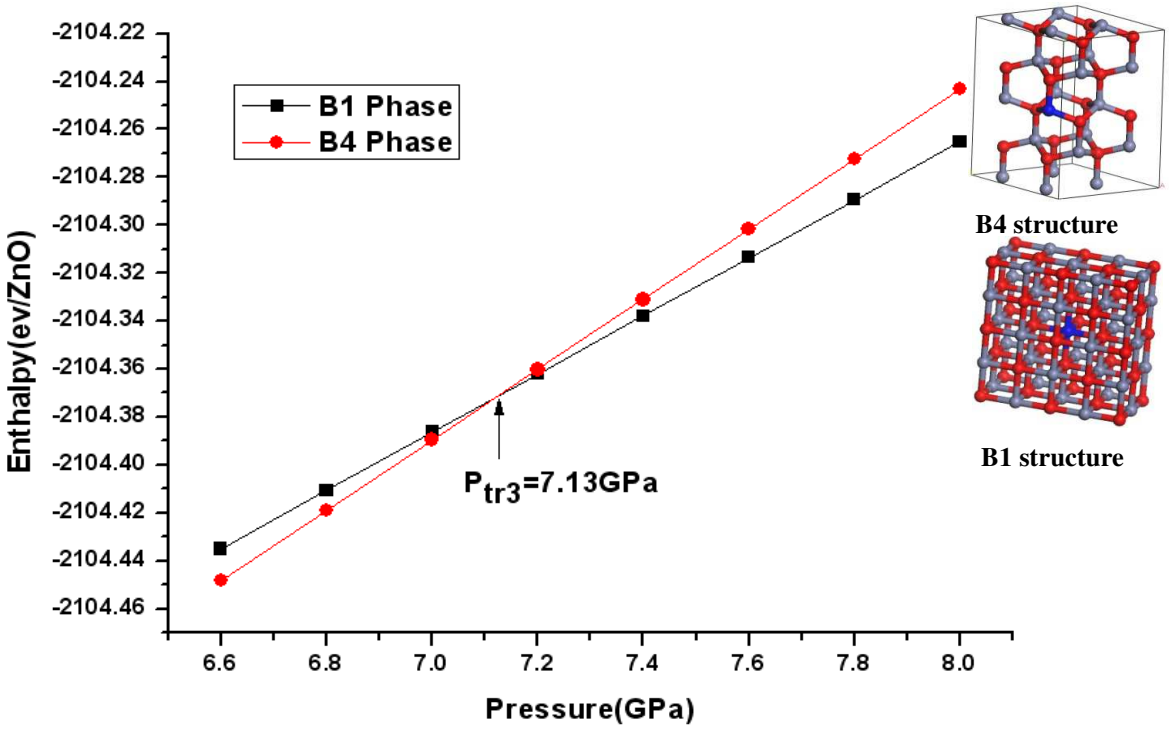

Figure S2. (a). The enthalpy as a function of pressure at temperature *T*=0 for B4 and B1 of Co-doped ZnO from calculations. The simulation cell includes 32 atoms, which is equivalent to a Co concentration of 6.25% ($Zn_{15}Co_1O_{16}$). The picture shows more than 32 atoms in the cell since the atoms on the surface and the corner are shared by adjacent cells;

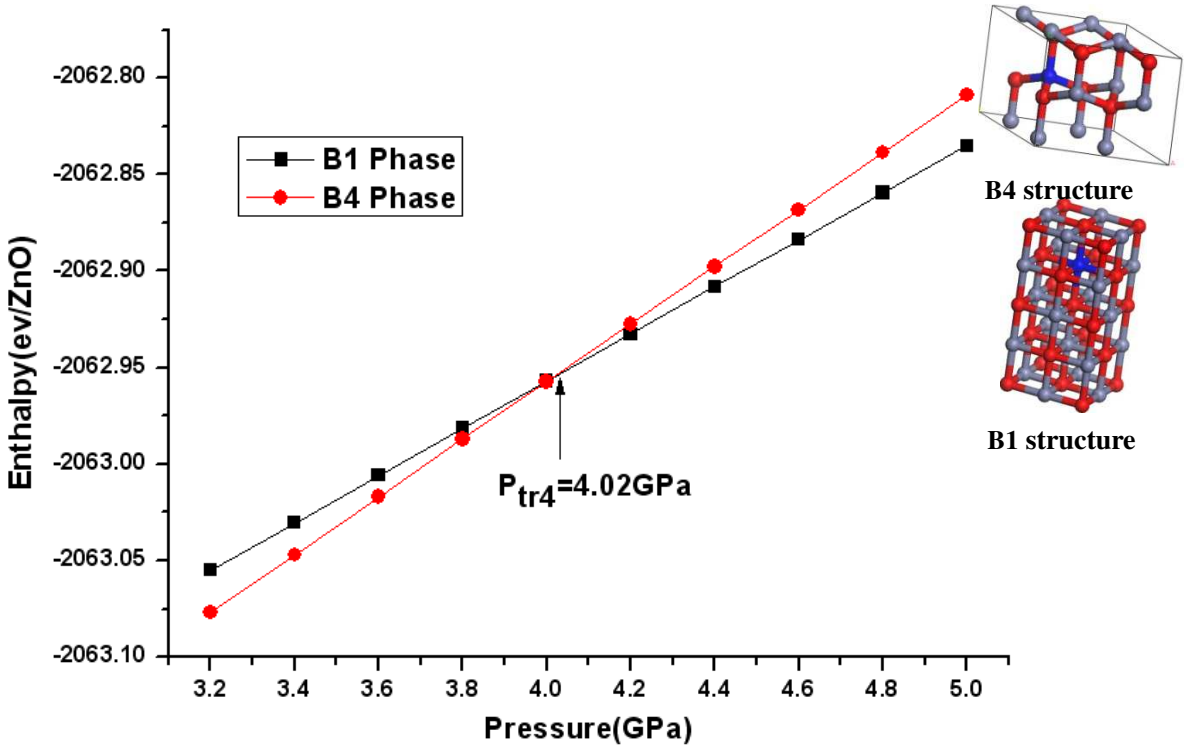

Figure S2 (b). The enthalpy as a function of pressure at temperature *T*=0 for B4 and B1 of Co-doped ZnO from calculations. The simulation cell includes 16 atoms, which is equivalent to a Co concentration of 12.5% ($Zn_7Co_1O_8$). The picture shows more than 16 atoms in the cell since the atoms on the surface and the corner are shared by adjacent cells.

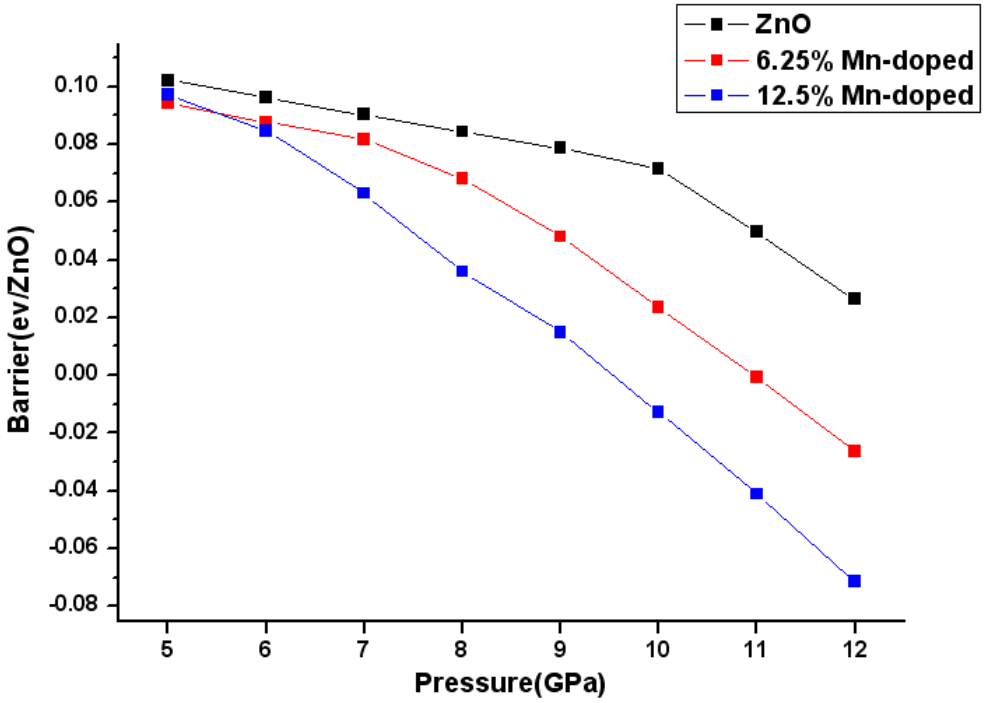

Figure S3 (a). The enthalpy transition barrier from B4 to B1 as a function of pressure for ZnO, 6.25% Mn-doped ZnO, and 12.5% Mn-doped ZnO.

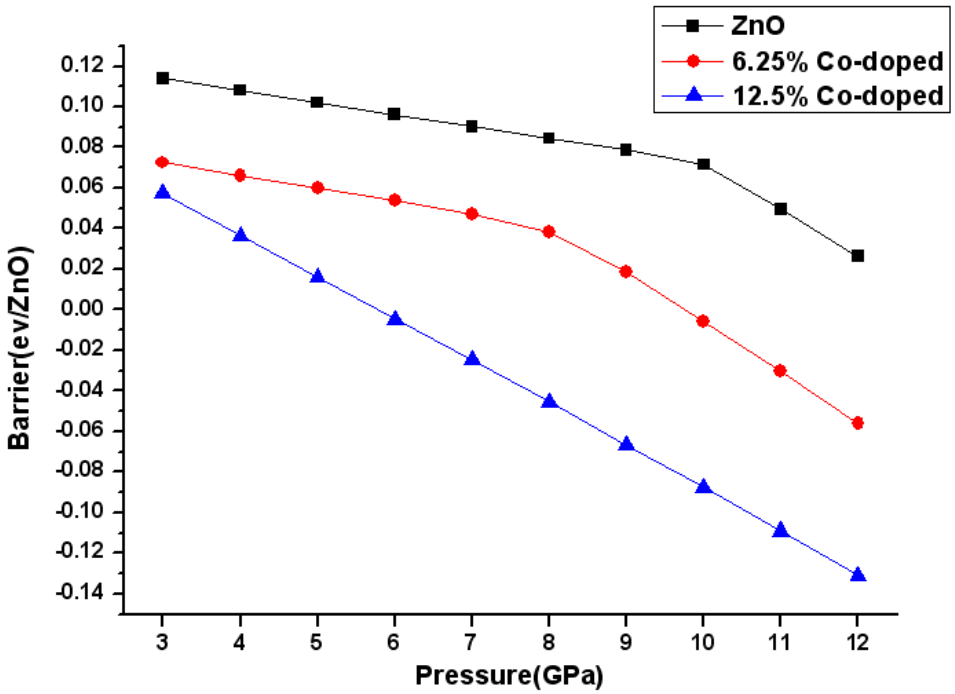

Figure S3 (b). The enthalpy transition barrier from B4 to B1 as a function of pressure for ZnO, 6.25% Co-doped ZnO, and 12.5% Co-doped ZnO.