Understanding the Role of Rare-Earth Metals Doping on the Electronic Structure and Optical Characteristics of ZnO

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Supporting Information

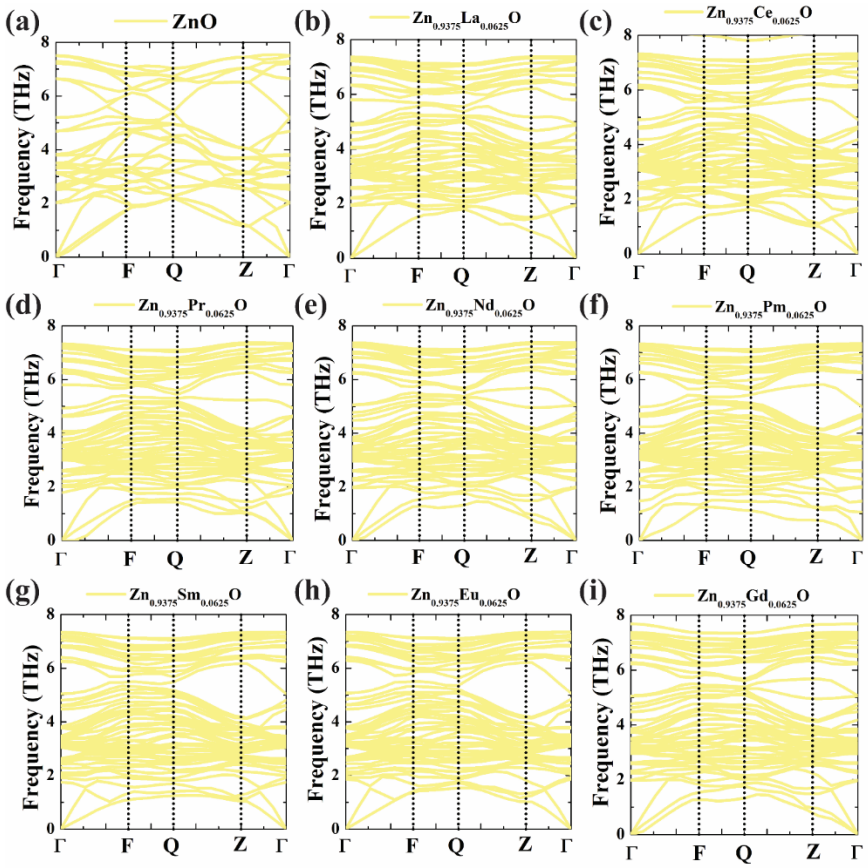

Figure S1. Phonon dispersion relation along the high symmetry Brillouin zone of (a) pure ZnO, (b) $Zn_{1-x}La_xO$ (c) $Zn_{1-x}CeO$ (d) $Zn_{1-x}Pr_xO$ (e) $Zn_{1-x}Nd_xO$ (f) $Zn_{1-x}Pm_xO$ (g) $Zn_{1-x}Sm_xO$ (h) $Zn_{1-x}Eu_xO$ and (i) $Zn_{1-x}Gd_xO$.

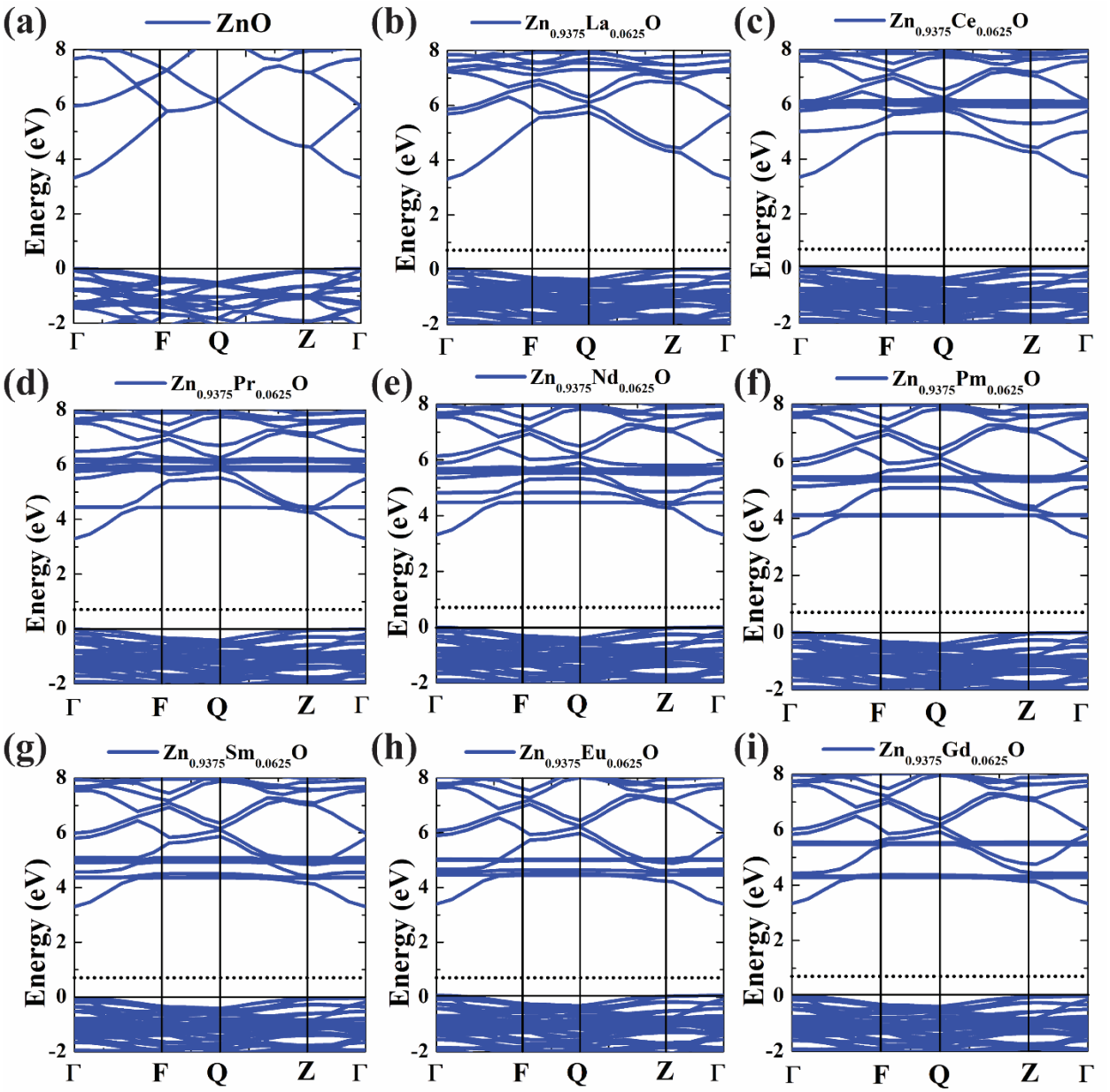

Figure S2. Electronic band structure from GGA+U calculations of (a) pure ZnO, (b) $Zn_{1-x}La_xO$ (c) $Zn_{1-x}CeO$ (d) $Zn_{1-x}Pr_xO$ (e) $Zn_{1-x}Nd_xO$ (f) $Zn_{1-x}Pm_xO$ (g) $Zn_{1-x}Sm_xO$ (h) $Zn_{1-x}Eu_xO$ and (i) $Zn_{1-x}Gd_xO$. CBM of bulk ZnO is noted by the black dotted line.

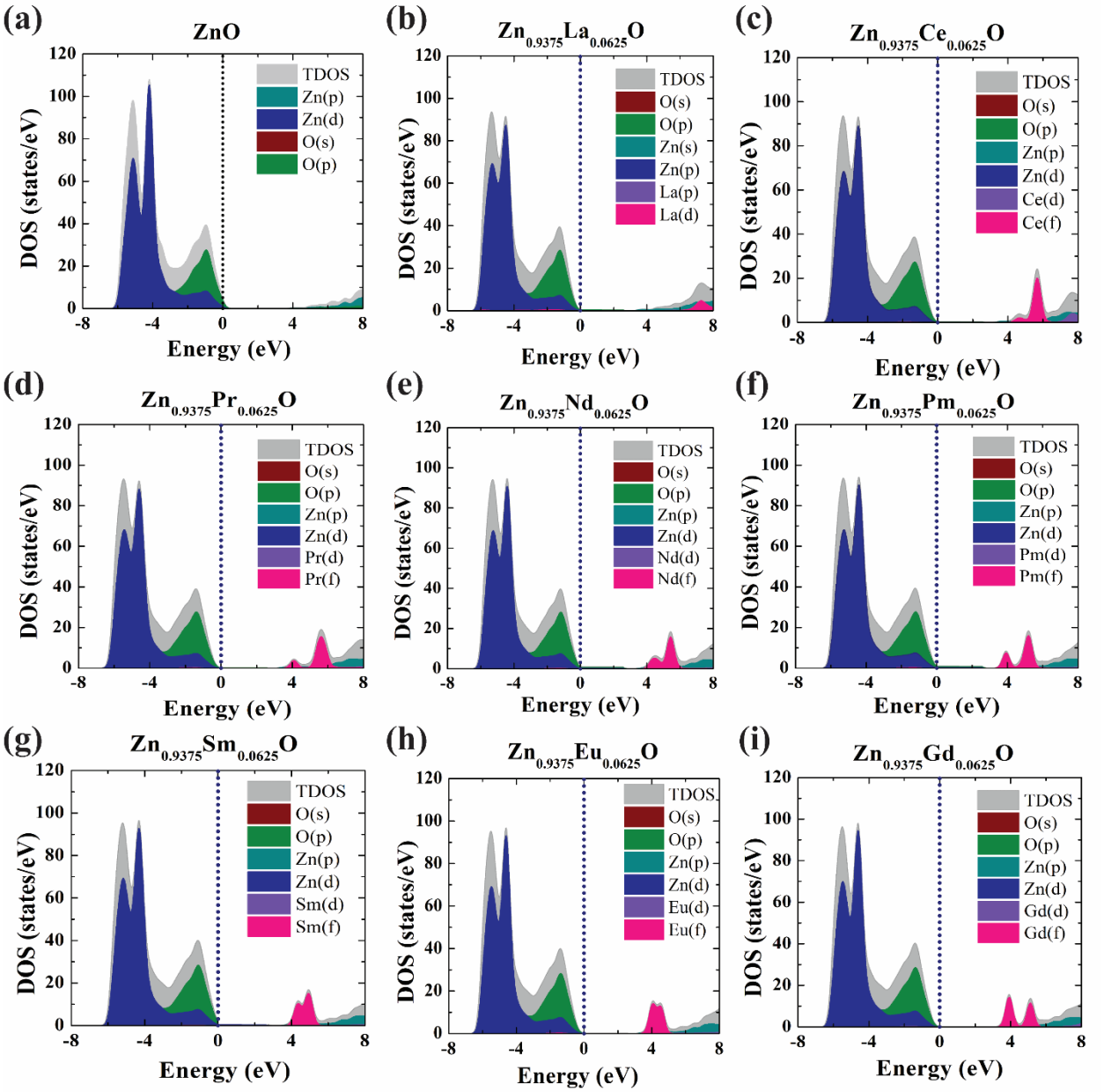

Figure S3. Electronic density of states from GGA+U calculations of (a) pure ZnO, (b) $Zn_{1-x}La_xO$ (c) $Zn_{1-x}CeO$ (d) $Zn_{1-x}Pr_xO$ (e) $Zn_{1-x}Nd_xO$ (f) $Zn_{1-x}Pm_xO$ (g) $Zn_{1-x}Sm_xO$ (h) $Zn_{1-x}Eu_xO$ and (i) $Zn_{1-x}Gd_xO$.

Optimized geometries in CIF format

Optimized geometries of RE doped ZnO using GGA theory have been added to the following GitHub repository **https://github.com/msehabibur/The-Role-of-Rare-Earth-Metals-Doping-on-the-Electronic-Structure-and-Optical-Characteristics-of-ZnO**