Explorations of new second-order NLO materials in the K^{I}-M^{II}-I^{V}-O systems

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Supporting Information

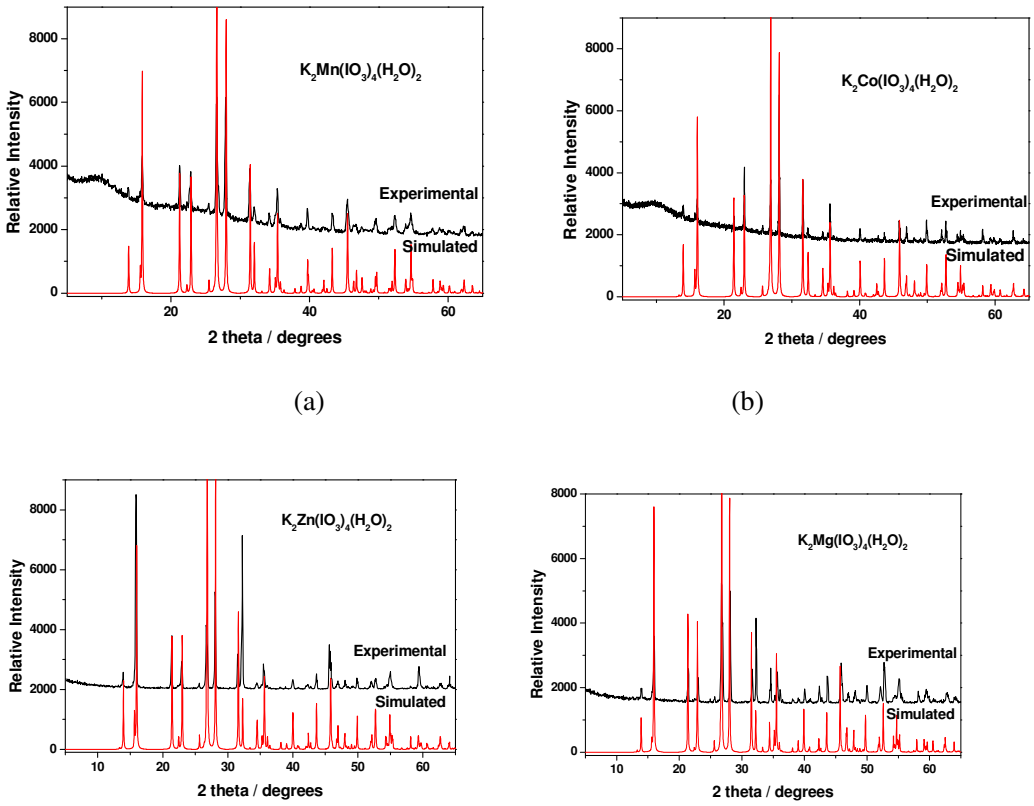


Figure S1. Simulated and experimental XRD powder patterns for $K_2M(IO_3)_4(H_2O)_2$ (M = Mn, Co, Zn, Mg).

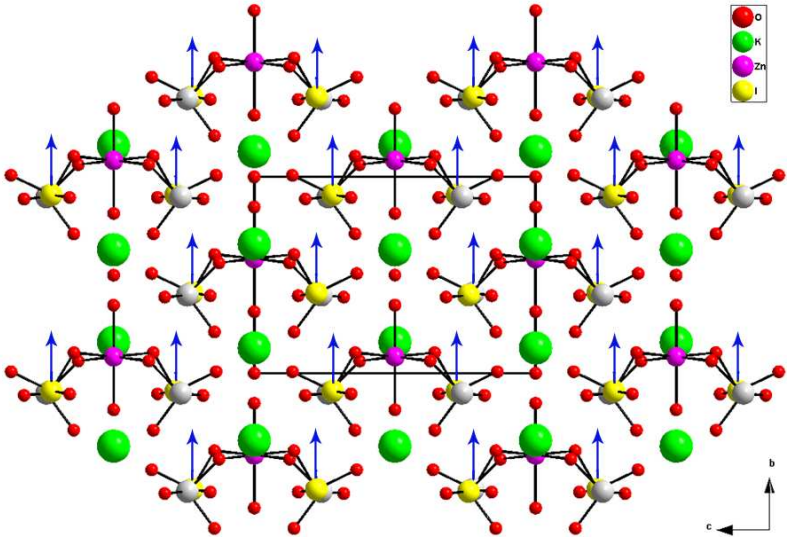


Figure S2. View of the structure of $K_2Zn(IO_3)_4(H_2O)_2$ along the *a* axis. K, Zn, I(1), I(2) and O atoms are represented by green, pink, yellow, light grey and red circles, respectively. The polarization directions of the iodate groups are indicated by green arrows.

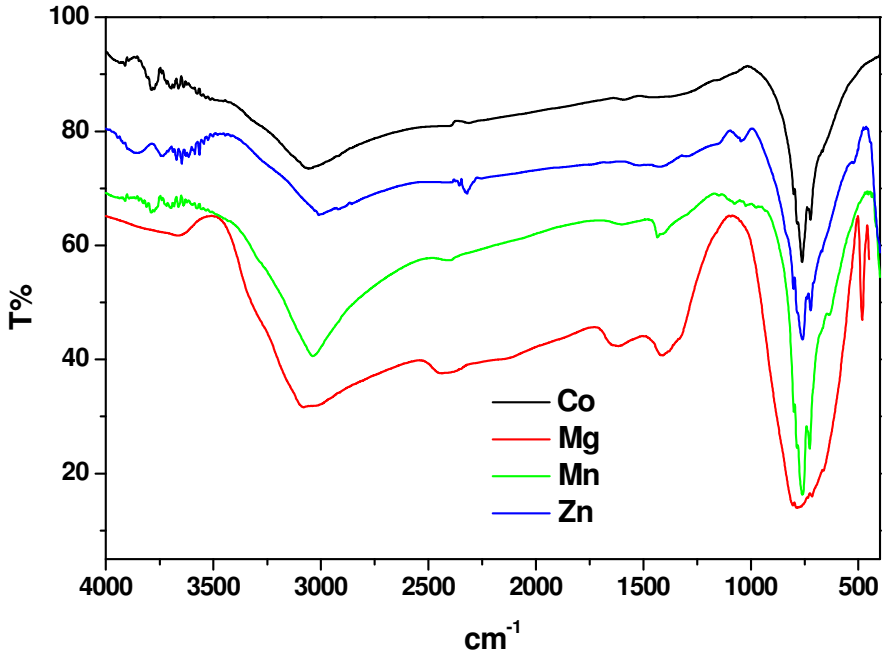


Figure S3. IR diagrams for $K_2M(IO_3)_4(H_2O)_2$ (M = Mn, Co, Zn, Mg).

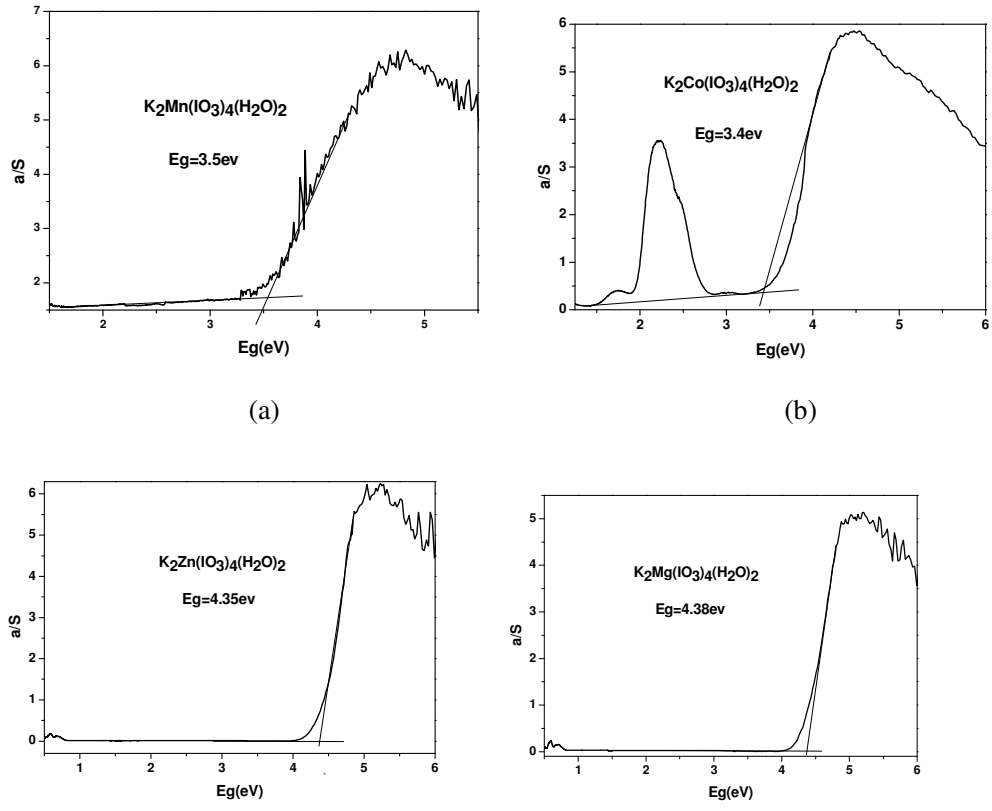


Figure S4. Optical diffuse reflectance spectra for $K_2M(IO_3)_4(H_2O)_2$ (M = Mn, Co, Zn, Mg).

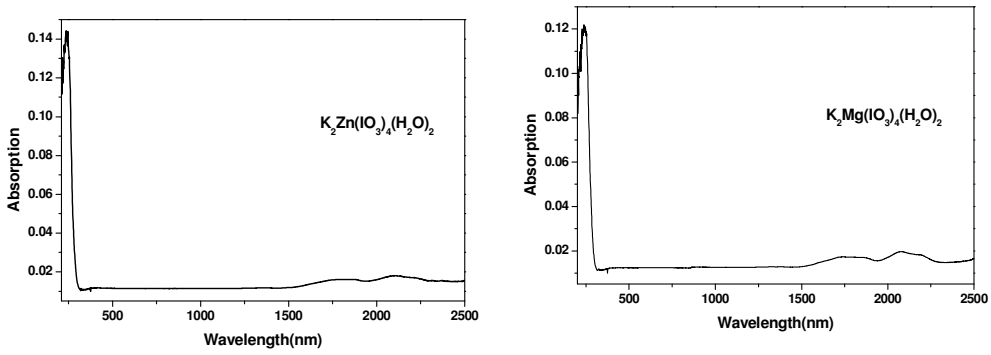


Figure S5. UV absorption spectrum for $K_2Zn(IO_3)_4(H_2O)_2$ (a) and $K_2Mg(IO_3)_4(H_2O)_2$ (b).

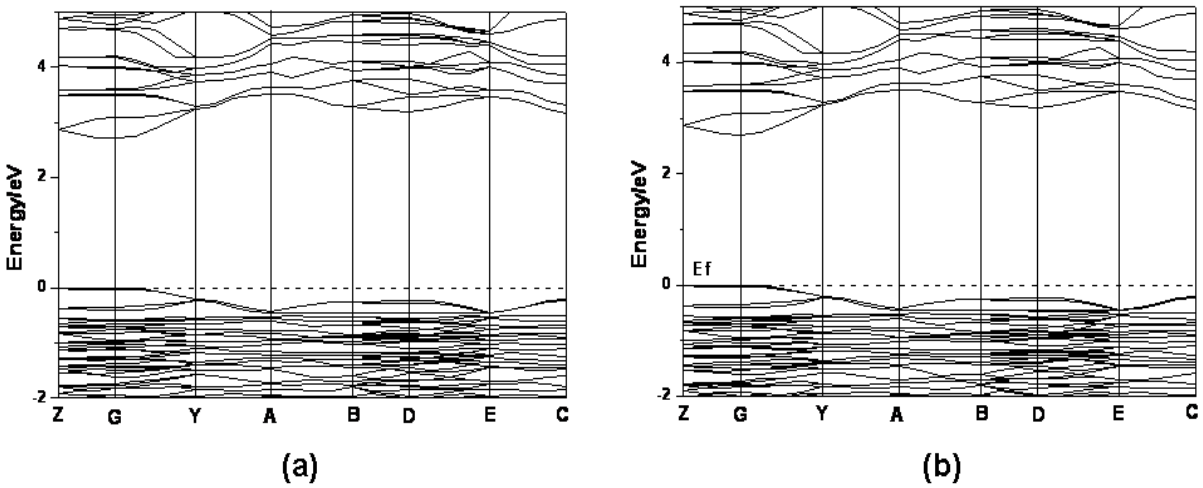
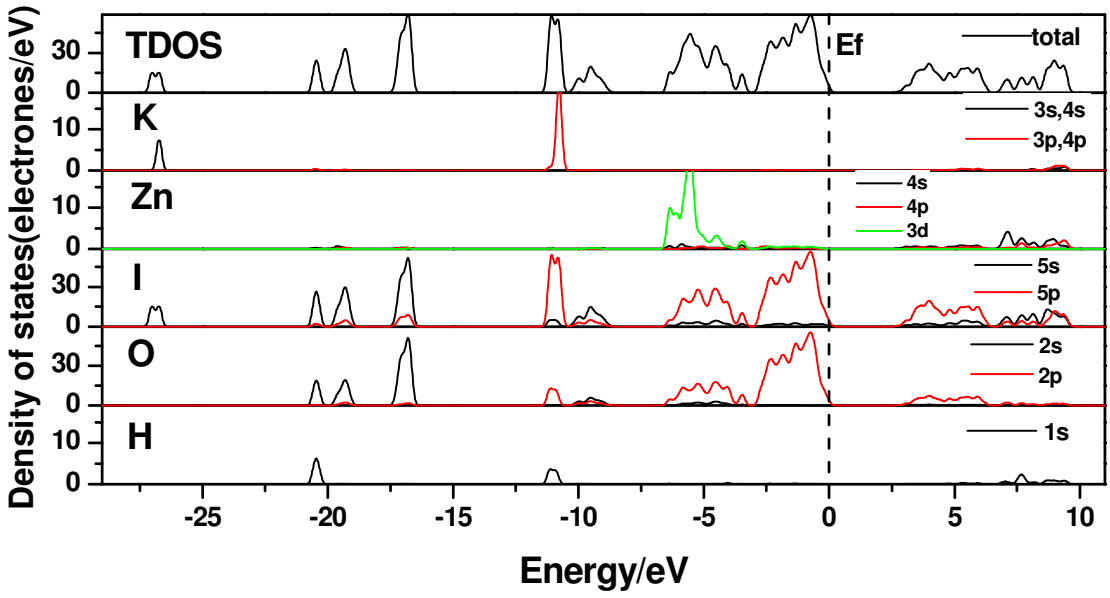
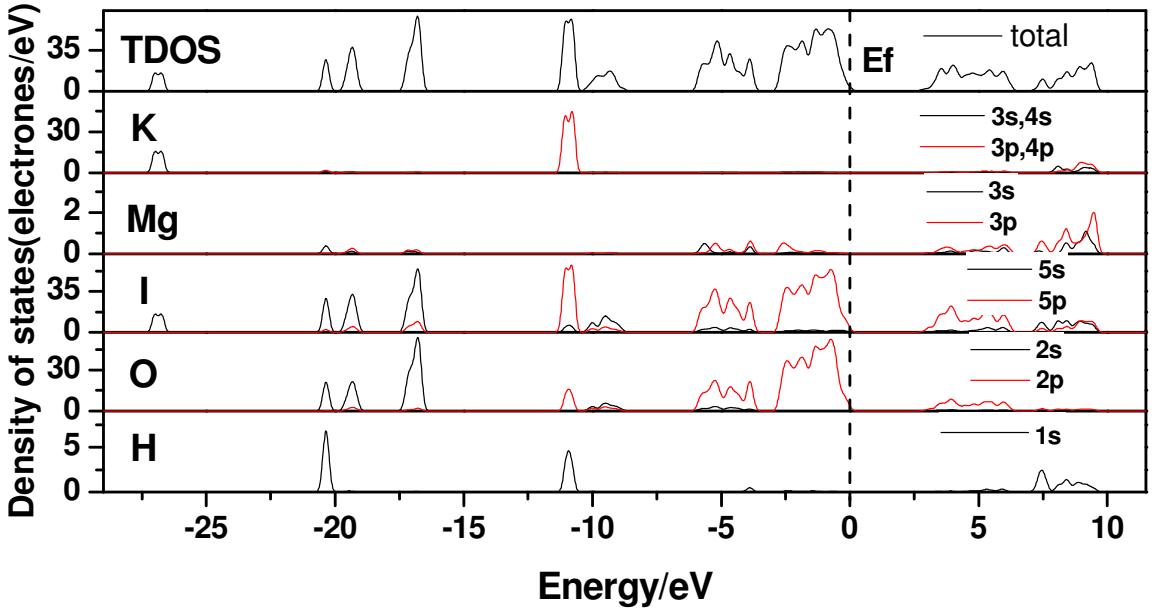


Figure S6. Band structures for $K_2Zn(IO_3)_4(H_2O)_2$ (a) and $K_2Mg(IO_3)_4(H_2O)_2$ (b). The Fermi level is set at 0 eV.

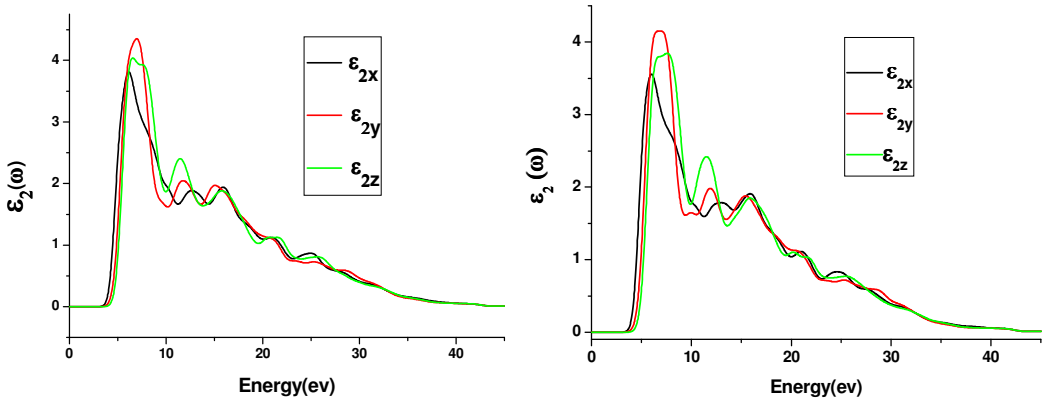


(a)



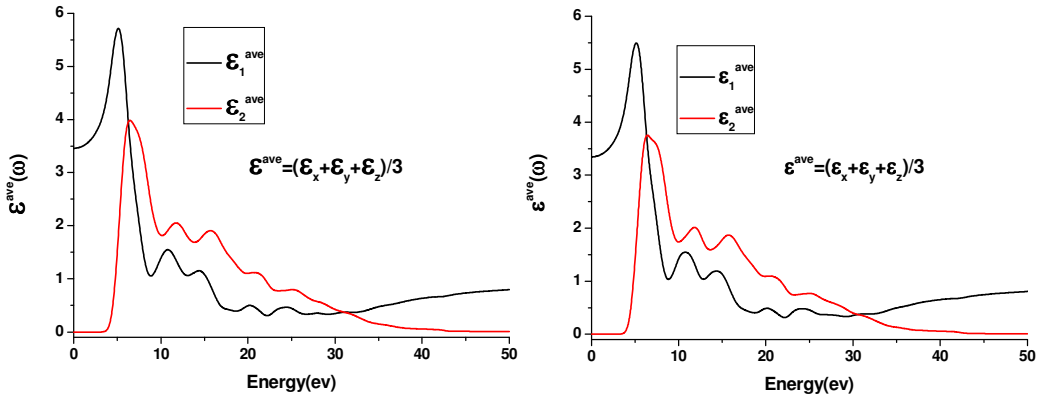
(b)

Figure S7. Total density of states and partial density of states of $K_2Zn(IO_3)_4(H_2O)_2$ (a) and $K_2Mg(IO_3)_4(H_2O)_2$. (b). The Fermi level is set at 0 eV.



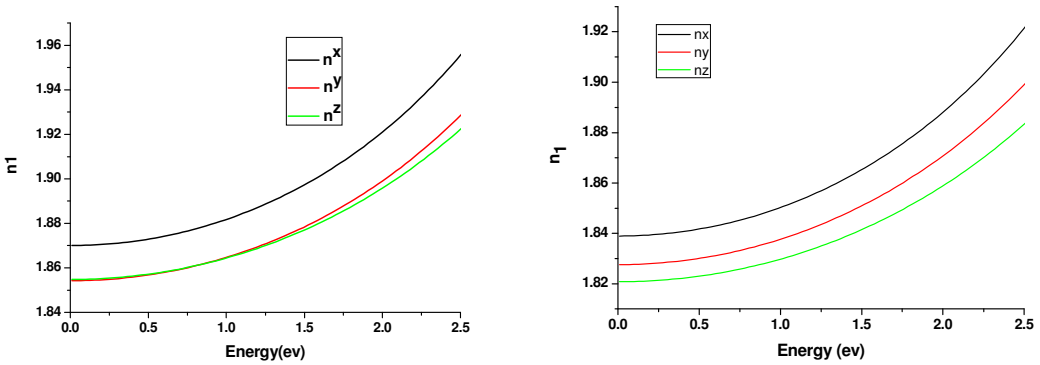
(a) (b)

Figure S8. The imaginary part of the dielectric function polarized along three dielectric axial directions and real part of the dielectric function over three dielectric axial directions for $K_2Zn(IO_3)_4(H_2O)_2$ (a) and $K_2Mg(IO_3)_4(H_2O)_2$ (b).



(a) (b)

Figure S9. The imaginary part of the dielectric function polarized along three dielectric axial directions and average imaginary part for $K_2Zn(IO_3)_4(H_2O)_2$ (a) and $K_2Mg(IO_3)_4(H_2O)_2$ (b).



(a) (b)

Figure S10. Calculated linear refractive indices for $K_2Zn(IO_3)_4(H_2O)_2$ (a) and $K_2Mg(IO_3)_4(H_2O)_2$ (b).

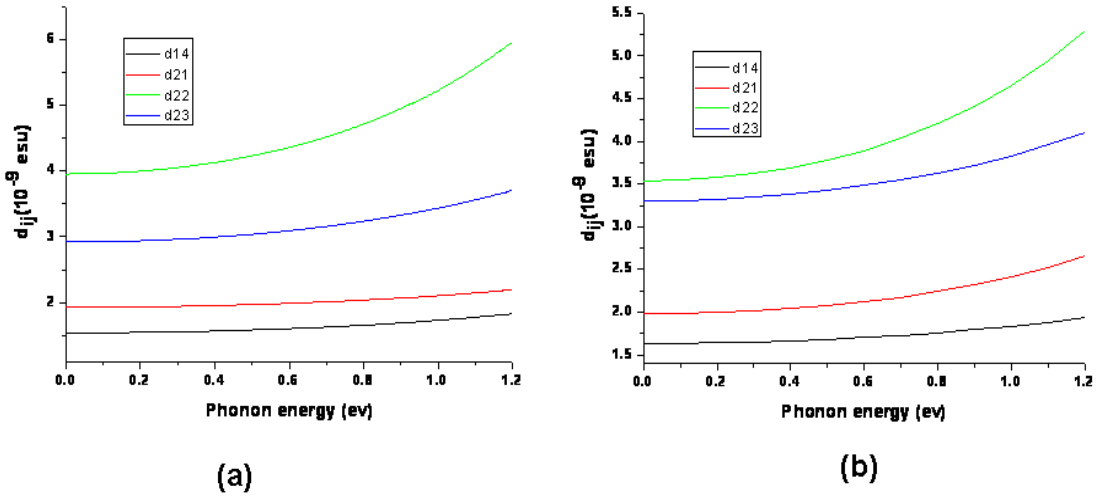


Figure S11. Calculated dynamic second harmonic generation coefficients of $K_2Zn(IO_3)_4(H_2O)_2$ (a) and $K_2Mg(IO_3)_4(H_2O)_2$ (b).