Second Harmonic Generation From the Novel Polar Polymorph α / β -$BaTeMo_2O_9$ Phases

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Supplementary materials

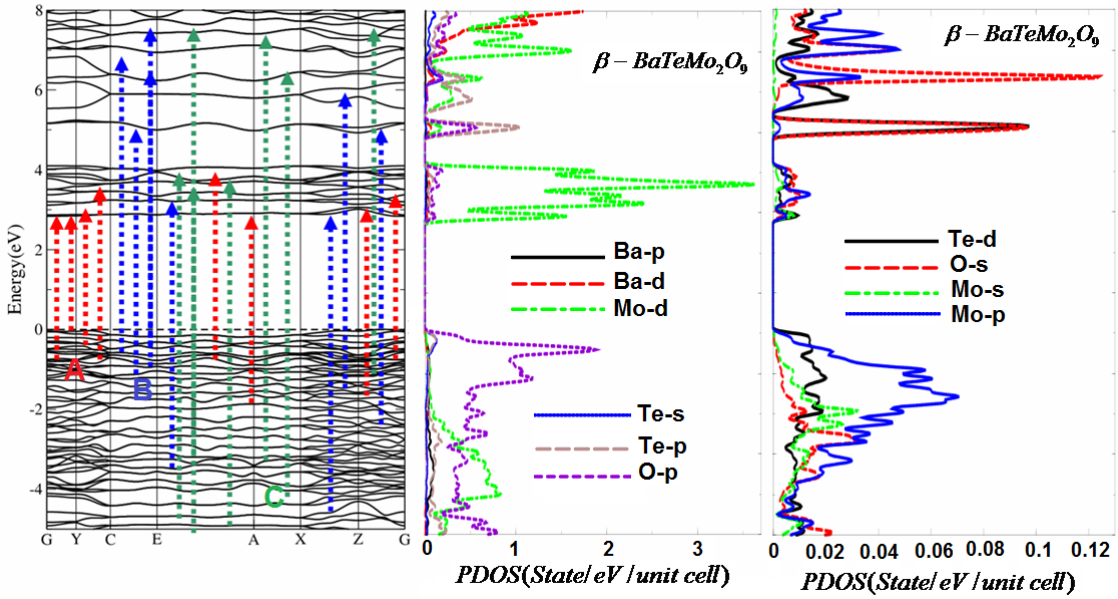

Fig. S: (a) The optical transitions depicted on a generic band structure of β-$BaTeMo_2O_9$ phase. For simplicity, we have labeled the optical transitions as A, B, and C. The transitions (A) are responsible for the structures for $\varepsilon_2^{xx}(\omega)$, $\varepsilon_2^{yy}(\omega)$ and $\varepsilon_2^{zz}(\omega)$ in the spectral range 0.0 -5.0 eV; the transitions (B) 5.0-10.0 eV , and the transitions (C) 10.0 - 14.0 eV. The electronic band structure and the associated partial density of states suggests that the first spectral structure in $\varepsilon_2^{xx}(\omega)$, $\varepsilon_2^{yy}(\omega)$ and $\varepsilon_2^{zz}(\omega)$ is due to the transition from O-s/p, Te-s/p/d, Ba-s and Mo-s/p states to Te-s/p/d, O-s/p, Ba-s and Mo-s/p states. The second structure corresponds to transition between Mo-s/p/d, Ba-s, O-s/p, Te-s/p/d states and O-s/p, Te-s/p/d, Ba-s/d, Ta-s/p/d states.

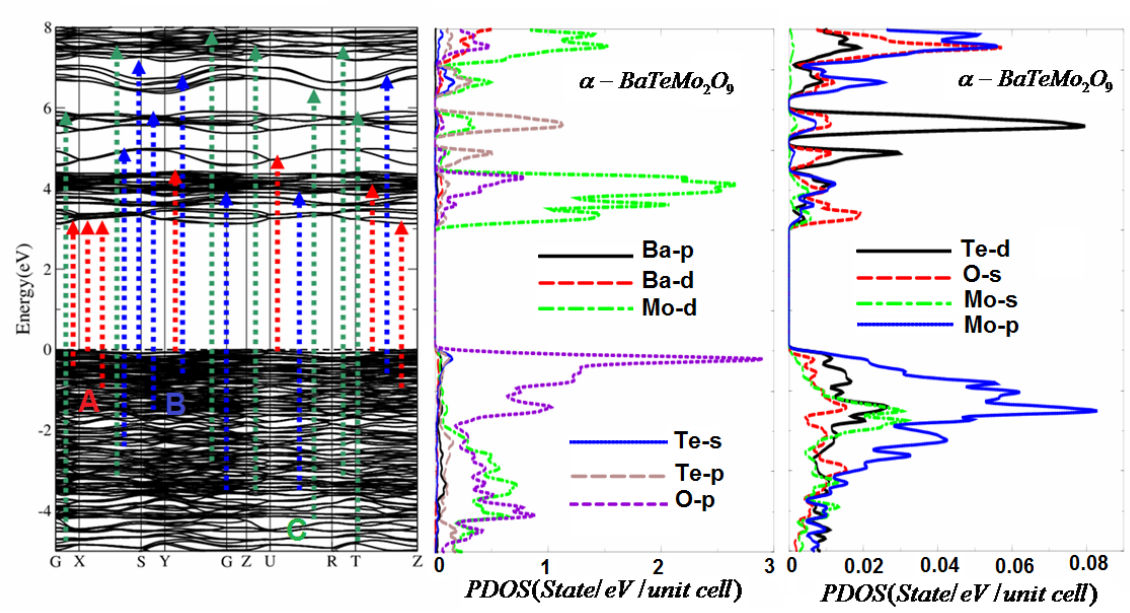

Fig. S: (b) The optical transitions depicted on a generic band structure of α-$BaTeMo_2O_9$ phase. For simplicity, we have labeled the optical transitions as A, B, and C. The transitions (A) are responsible for the structures for $\varepsilon_2^{xx}(\omega)$, $\varepsilon_2^{yy}(\omega)$ and $\varepsilon_2^{zz}(\omega)$ in the spectral range 0.0 -5.0 eV; the transitions (B) 5.0-10.0 eV , and the transitions (C) 10.0 - 14.0 eV. The electronic band structure and the associated partial density of states suggests that the first spectral structure in $\varepsilon_2^{xx}(\omega)$, $\varepsilon_2^{yy}(\omega)$ and $\varepsilon_2^{zz}(\omega)$ is due to the transition from O-s/p, Te-s/p/d, Ba-s and Mo-s/p states to Te-s/p/d, O-s/p, Ba-s and Mo-s/p states. The second structure corresponds to transition between Mo-s/p/d, Ba-s, O-s/p, Te-s/p/d states and O-s/p, Te-s/p/d, Ba-s/d, Ta-s/p/d states.