Electronic Supplementary Information for

High-pressure dielectric behavior of $BaMoO_4$: A combined experimental and theoretical study

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Supplementary Material

$BaMoO_4$ powder with purity of 99.9% was bought from the Alfa Aesar Co. The initial structure of the sample was the tetragonal structure (space group I41/a), and has been confirmed by a powder X-ray diffractometer with Cu-Kα radiation. Figure S1 gives the XRD spectrum.

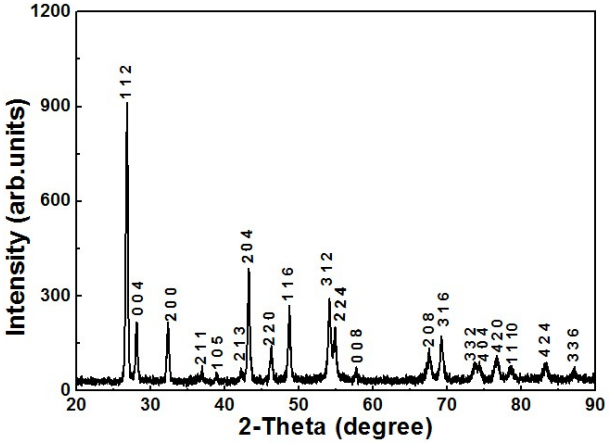

Figure S1. X-ray diffraction pattern of the $BaMoO_4$ sample at ambient pressure.

The energy band structures of the tetragonal and monoclinic phase were calculated at different pressures by the first-principles calculations, the variation tendency of band gap (E_g) along with pressure was obtained. In Table S1, We make a comparation between dE_g/dP and d(ln$R$)/d(P) through the following Arrhennius relationship.

$$d(lnR)/dP = (1/2k_BT)(dE_g/dP), \quad \text{(S1)}$$

where R is the resistance received from the experiment, E_g represents the band gap received from the theoretical calculations, k_B is the Boltzmann constant, and T represents room temperature. The result indicates that the effect of pressure on the band gap did not play a vital role in the two phases. Therefore, we contend that the growth of R is mainly caused by the increasing defect levels, and the lattice scattering was enhanced.

Table S1. The pressure dependence of E_g and ln$R$ for the first two phases of $BaMoO_4$

Phase	Pressure region (GPa)	$(2k_BT)^{-1}dE_g/dP$ (GPa^{-1}) (theoretical)	$d(\ln R)/dP$ (GPa^{-1}) (experimental)
Tetragonal	1.9～4.8	0.02	0.05
Monoclinic	4.8～8.8	0.01	0.14