

Supplementary Information (SI)

High-pressure Band-Gap Engineering and Structural Properties of the van der Waals BiOCl Nanosheets

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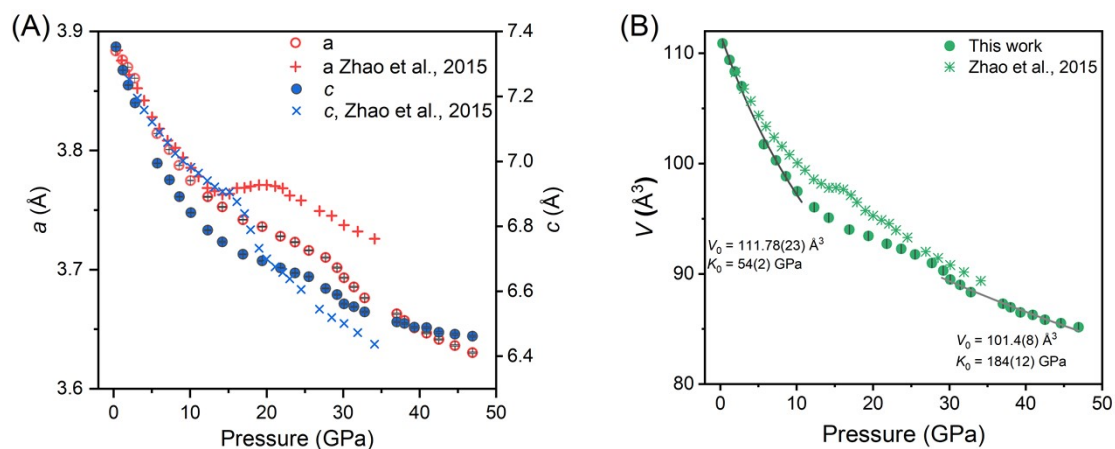


Fig. S1 (A) Lattice parameters of a (red symbols) and c (blue symbols). (B) Experimental volume evolution with pressure. The determined equations of state (gray solid lines) by the 2nd order Birch-Murnaghan equation of state (BM2-EoS). V_0 and K_0 correspond volume and bulk modulus at ambient condition, respectively. The crosses and stars represent data from Zhao et al., 2015.¹

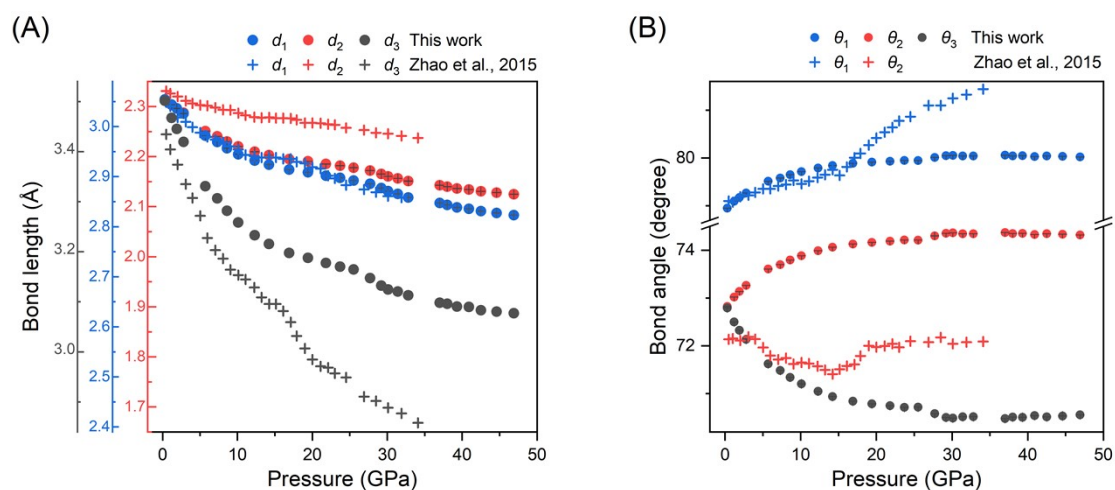


Fig. S2 (A) Evolution of Bi-O and Bi-Cl bond lengths under compression. The relative values of the right and left axes are consistent. (B) Bond angles evolution of Cl-Bi-Cl, O-Bi-O and O-Bi-Cl, respectively. The crosses and stars represent data from Zhao et al., 2015.¹

1. J. Zhao, L. Xu, Y. Liu, Z. Yu, C. Li, Y. Wang and Z. Liu, *The Journal of Physical Chemistry C*, 2015, **119**, 27657-27665.