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CORRECTION

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Correction: Topological behaviour of ternary non-symmorphic crystals KZnX (X = P, As, Sb) under pressure and strain: a first principles study

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Correction for 'Topological behaviour of ternary non-symmorphic crystals KZnX (X = P, As, Sb) under pressure and strain: a first principles study' by Atahar Parveen *et al.*, *Phys. Chem. Chem. Phys.*, 2018, **20**, 5084–5102.

Unfortunately, in the original article,[1] for the ground state of KZnAs a band gap calculated with GGA was reported as the TBmBJ band gap and one with GGA + SO was reported as the TBmBJ + SO band gap. To correct this, changes in Table 1 and Fig. 2(b), 3(b), 4(b) and 7(b) are presented below. The overall results and conclusions remain unaffected as the error is related only to the ground state band gap of KZnAs.

Table 1 Optimized structural parameters of ternary KZnAs, band gap (E_g) with (GGA + TBmBJ) and with SOC data

Compound	a (Å)	c (Å)	V (Å^3)	E_g (eV)	With SOC (eV)
KZnAs	4.270	10.36	163.65	1.363	1.288

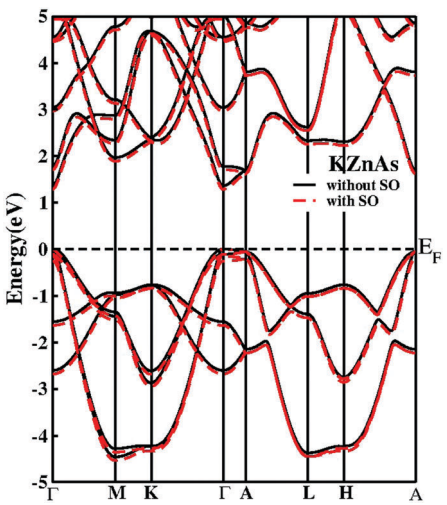

Fig. 2 (b) Calculated band structure using the TB-mBJ functional without and with SO interaction in the ground state for KZnAs at the theoretical volume.

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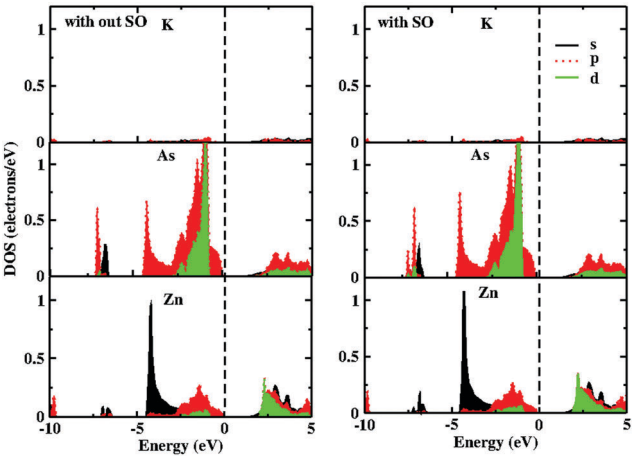

Fig. 3 (b) Calculated partial density of states using TB-mBJ without and with SO interaction in the ground state for KZnAs.

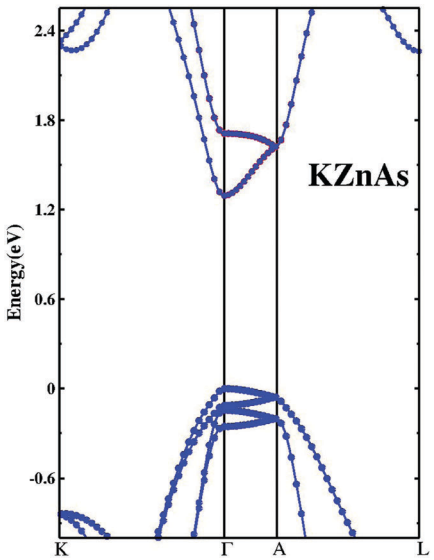

Fig. 4 (b) Calculated s and p projected band structures with the inclusion of SOC for KZnAs Each red and blue dot size quantifies the weight of Zn-s and As-p orbitals respectively.

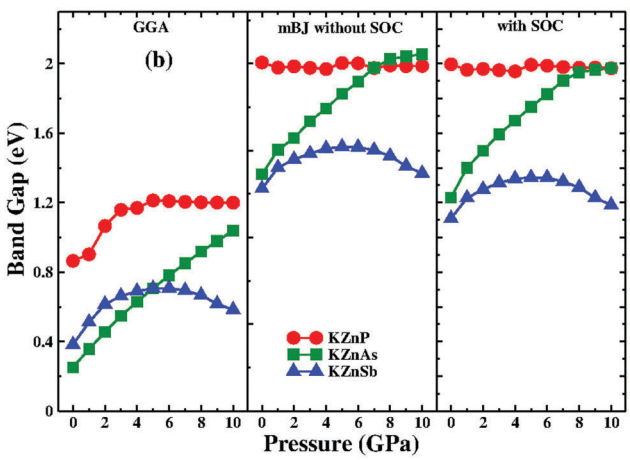

Fig. 7 Calculated band gap obtained for KZnX when GGA, TB-mBJ functionals were employed without and with the inclusion of SOC up to 10 GPa.

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

References

1 A. Parveen, E. Narsimha Rao, B. Adivaiah, P. Anees and G. Vaitheeswaran, Topological behaviour of ternary nonsymmorphic crystals KZnX (X = P, As, Sb) under pressure and strain: a first principles study, *Phys. Chem. Chem. Phys.*, 2018, **20**, 5084–5102.