Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

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

T. Atahar Parveen,*,† E. Narsimha Rao,† B. Adivaiah,† P. Anees,‡ and G. Vaitheeswaran*,†

Advanced Center of Research in High Energy Materials (ACRHEM), University of Hyderabad, Prof. C. R. Rao Road, Gachibowli, Hyderabad-500 046, Telangana, India, and Materials Physics Division, Indira Gandhi Centre for Atomic Research, Kalpakkam, 603102, India

E-mail: ataharparveen@gmail.com; vaithee@uohyd.ac.in

*To whom correspondence should be addressed

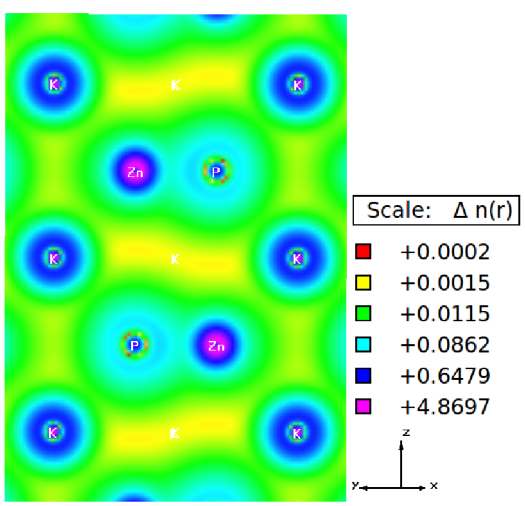
†Advanced Center of Research in High Energy Materials (ACRHEM), University of Hyderabad, Prof. C. R. Rao Road, Gachibowli, Hyderabad-500 046, Telangana, India

‡Materials Physics Division, Indira Gandhi Centre for Atomic Research, Kalpakkam, 603102, India

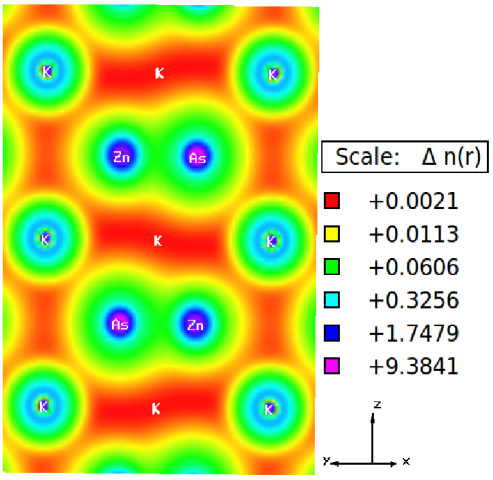
Table 1: Bond distances of KSbZn at ambient conditions compared with experimental results

Compound	Bonds	This work (Å)	Exp.(Å)
KZnP	K-K	4.10	4.09[1]
	K-P	3.55	3.46[1]
	K- Zn	3.55	3.46[1]
	P-Zn	2.36	2.36[1]
KZnAs	K-K	4.27	4.22[2]
	K-As	3.69	3.53[2]
	K-As	3.69	3.53[2]
	As-Zn	2.46	2.43[2]
KZnSb	K-K	4.59	4.54[1]
	K-Sb	3.76	3.71[1]
	K-Zn	3.76	3.71[1]
	Sb-Zn	2.65	2.62[1]

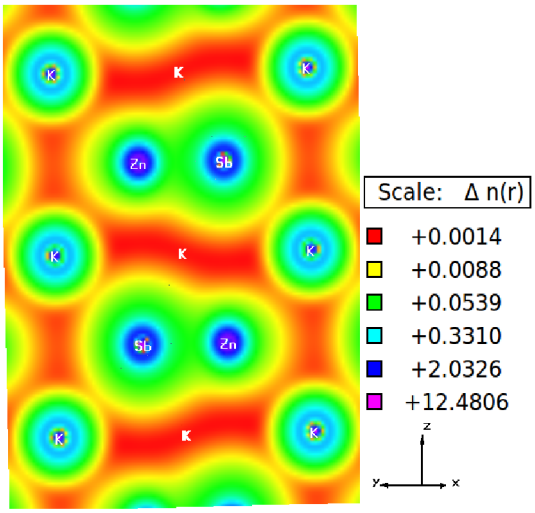
.



(a)



(b)



(c)

Figure 1: (Color online)Contour plot of charge density plots for (a) KZnP (b) KZnAs (c) KZnSb crystals.

References

(1) Gerhard Savelsberg and Herbert Schfer, Z. Naturforsch. 33B, 370-373 (1978)

(2) Rainer Vogel and Hans-Uwe Schuster, Z. Naturforsch. 85B, 114-116 (1980)