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Electronic Supplementary Material

Influence of defect distribution on the thermoelectric properties of FeNbSb based materials

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Table S1: Effective cluster interactions (ECI) (meV/atom) for $FeNb_{1-x}V_xSb$ and $FeNb_{1-x}Ti_xSb$. The triplets are identify according to their longest side, the other two sides being the first-nearest neighbors.

Cluster	1st pair	2nd pair	3rd pair	4th pair	1st triplet	2nd triplet
$FeNb_{1-x}V_xSb$	-3.1	0.8	-0.4	0.1	-0.4	-0.1
$FeNb_{1-x}Ti_xSb$	0.3	0.6	-0.8	-0.4	-1.6	-0.4

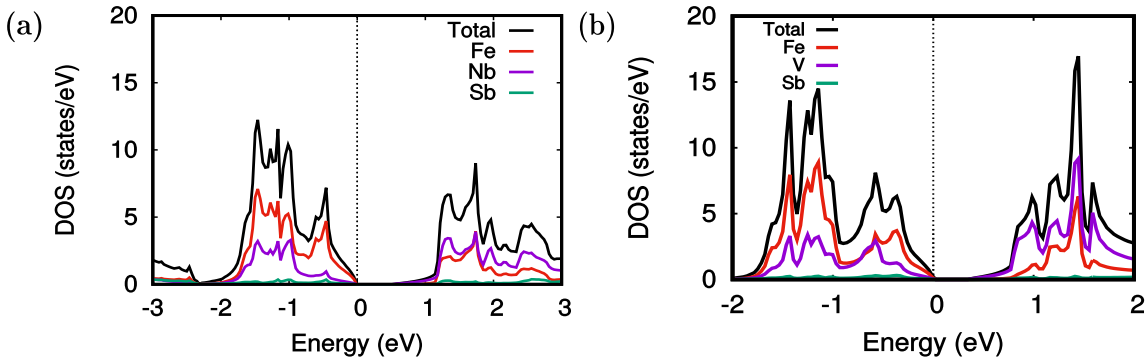

Fig. S1: The total and partial density of states of FeNbSb (a) and FeVSb (b).

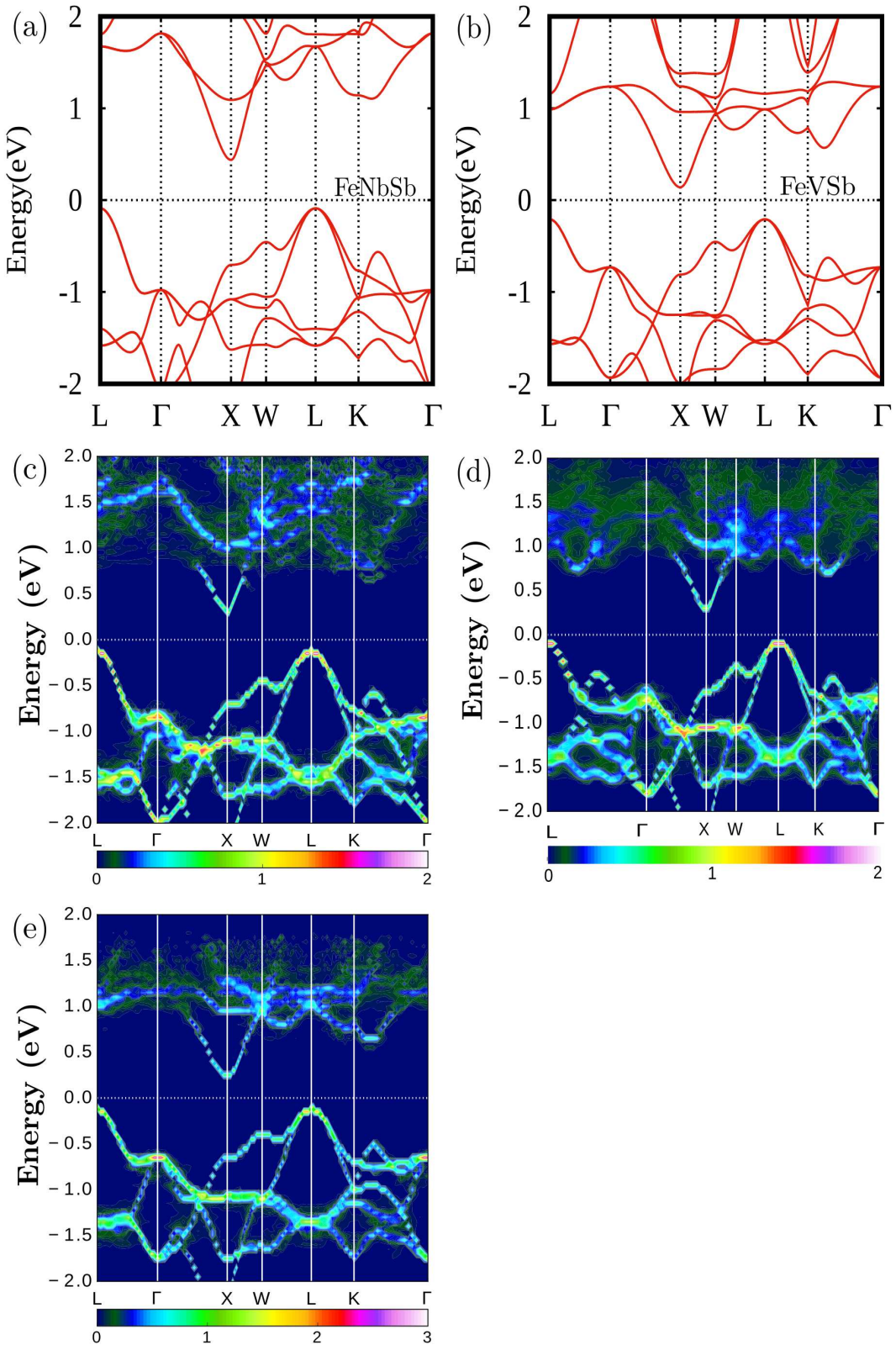

Fig. S2: The band structures of pristine compounds FeNbSb (a), FeVSb (b), and three $FeNb_{1-x}V_xSb$ SQSs with x = 25 %(c), 50 % (d) and 75 %(e) after band unfolding.

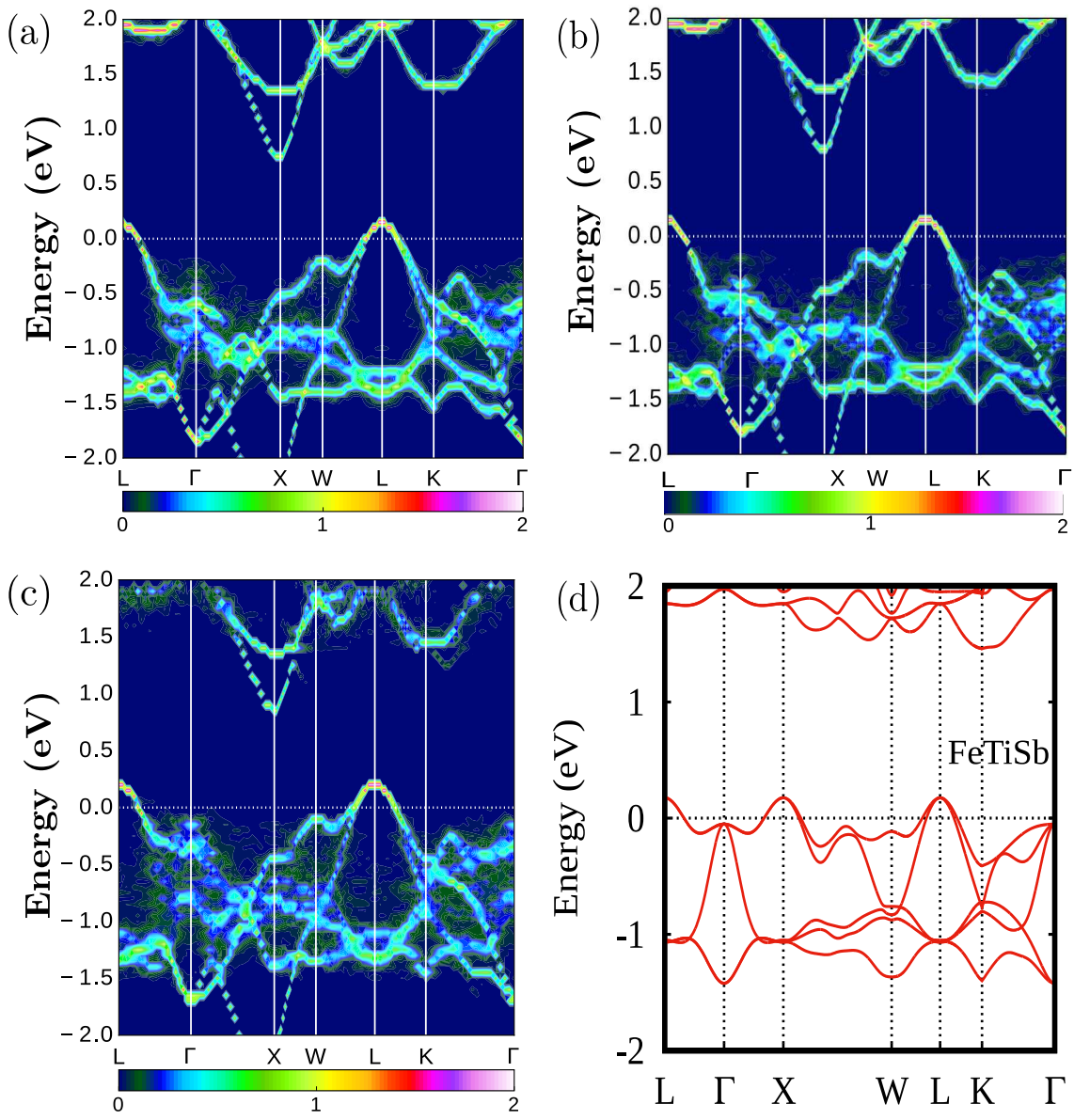

Fig. S3: The band structures of $FeNb_{1-x}Ti_xSb$: two theoretically predicted ground states $Fe_8Nb_7Ti_1Sb_8$ (a), $Fe_6Nb_5Ti_1Sb_6$ (b) and one SQS with $x = 25$ % (c) after band unfolding and FeTiSb (d).