High Temperature Thermoelectric Properties of the Solid-Solution Zintl Phase $Eu_{11}Cd_6Sb_{12-x}As_x$ ($x < 3$)

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Supporting Information

TGDSC data for $Eu_{11}Cd_6Sb_{12}$

38.0 mg of $Eu_{11}Cd_6Sb_{12-x}As_x$ x_{syn}=2 single crystals were used for TG-DSC analysis under Ar flow. The mass decreasing by 7.07% around 600 ˚C may attribute to As/Sb evaporation. TGDSC data of $Eu_{11}Cd_6Sb_{12}$ shows a mass loss around 650 ˚C which may be due to vaporization of Sb.

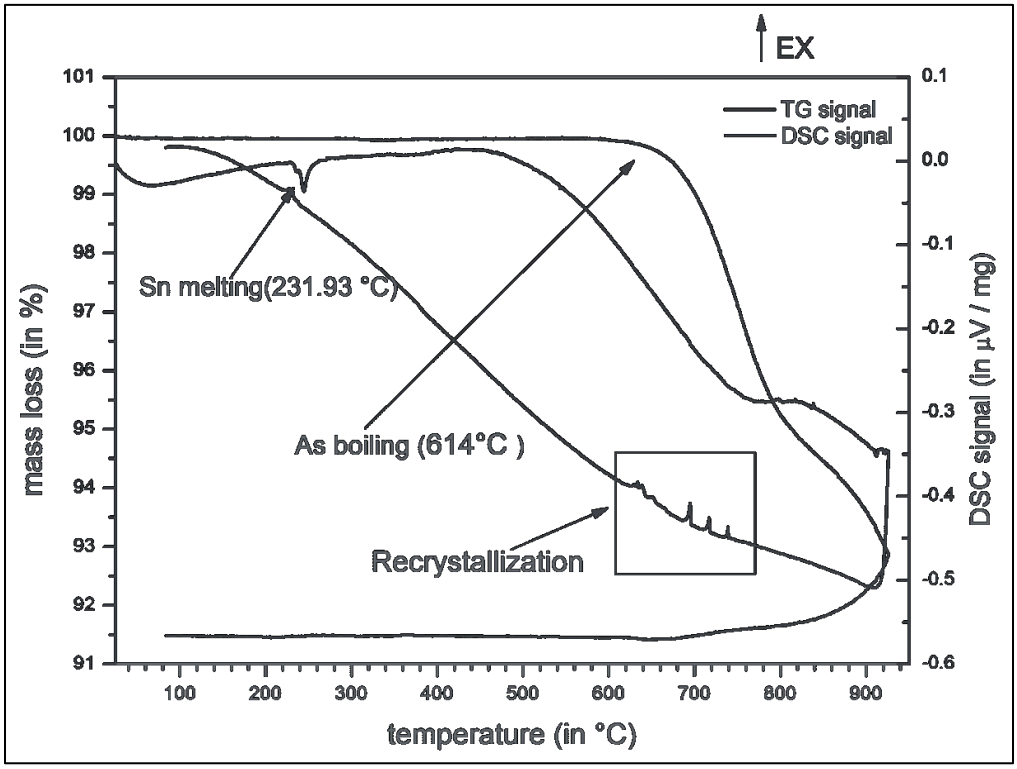

Figure S1. TG_DSC analysis show that there is a mass loss at around 600 which can be attributed to As evaporation.

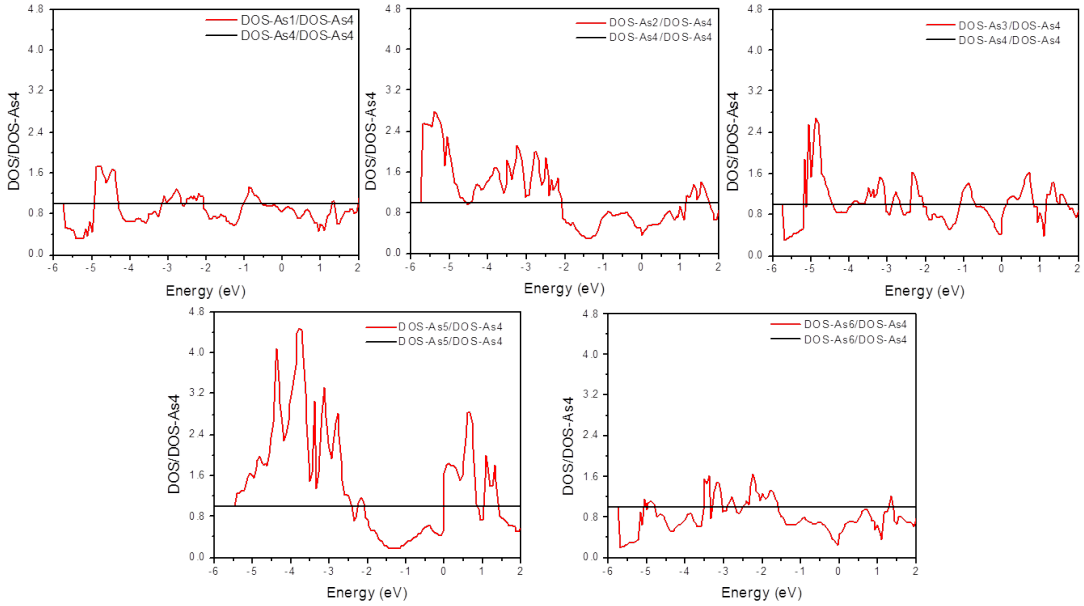

Figure S1. Ratios of As partial DOS curves for sites As1, As2, As3, As5, As6 with respect to the As4 site. The reference line in each graph is 1.00. When the curve lies above 1.00, the contribution to the DOS from the site exceeds that from As4; when the curve lies below 1.00, the contribution to the DOS from As4 exceeds that from the given site.

Table S2. Thermal Diffusivity Data for $Eu_{11}Cd_6Sb_{12-x}As_x$ (x=0, 1, and 2)

x = 0	Temp.	λ(W/mK)	x = 1	Temp.	λ(W/mK)	x = 2	Temp.	λ(W/mK)
	352.25	0.789942		353.75	0.822189		324.85	0.833746
	371.35	0.76849		373.75	0.80694		372.65	0.79669
	421.45	0.716753		423.65	0.763733		421.45	0.771987
	474.25	0.671325		473.95	0.724339		474.15	0.738637
	525.95	0.629682		523.95	0.663342		525.95	0.675643
	575.65	0.619587		574.05	0.658259		575.65	0.685524
	625.35	0.615802		624.05	0.655718		625.35	0.694171
	675.05	0.618325		674.05	0.655718		675.05	0.704052
	724.85	0.627159		724.05	0.669696		724.75	0.718874
	774.55	0.637254		774.05	0.682404		774.65	0.732461
	672.05	0.60823		673.55	0.645552		672.05	0.671937
	571.15	0.601921		573.35	0.629032		571.15	0.644763
	469.55	0.644825		473.35	0.684946		469.55	0.674408
	369.75	0.7483		373.65	0.766275		369.55	0.732461
	321.95	0.811394		323.45	0.815835		311.95	0.778163