The comparison of the Seebeck coefficients between the experimental and theoretical values.

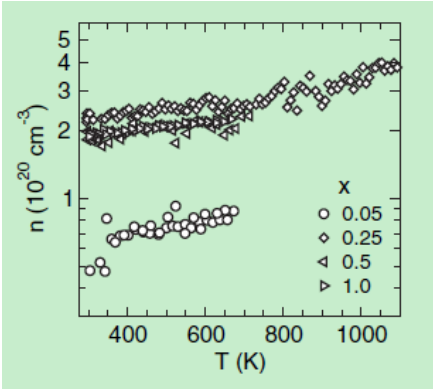

Fig. 1. The Hall Carrier concentration is constant with temperature for all $Ca_{5-x}Na_xAl_2Sb_6$ compositons, suggesting the successful formation of heavily doped semiconductor.

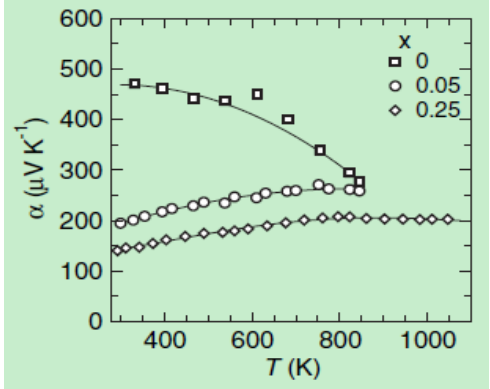

Fig. 2. Higure-temperature Seebeck coefficients of $Ca_{5-x}Na_xAl_2Sb_6$ show decreasing magnitude with increasing carrier concentration.

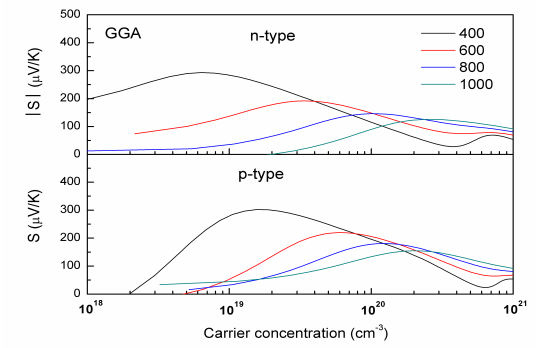

Fig. 3. Calculated Seebeck coefficients of $Ca_5Al_2Sb_6$ with GGA.

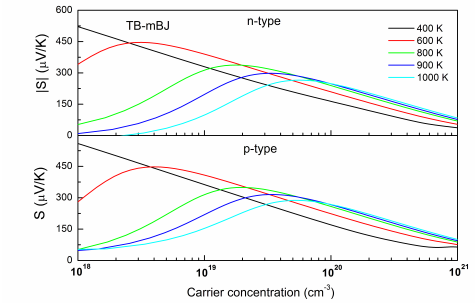

Fig. 4. Calculated Seebeck coefficients of $Ca_5Al_2Sb_6$ with TB-mBJ.

Fig. 1 and Fig. 2 are the experimental data in Ref. 20 (Advanced Functional Materials 20 (2010) 4375), which corresponds to the p-type doping. Fig. 3 and Fig. 4 are the theoretical values calculated by different exchange-correlation potentials. We list them in below table for comparison. We can see that the theoretical Seebeck coefficients calculated by TB-mBJ are more consistent with the experimental results.

Temperature (K)	Carriers concentration (cm^{-3})	Seebeck(experiment) (μV/K)	Seebeck (GGA) (μV/K) p-type	Seebeck(TB-mBJ) (μV/K) p-type
400	x=0	460	300(biggest)	566(biggest)
400	6.6×10^{19} (x=0.05)	210	230	207
400	2.3×10^{20}(x=0.25)	160	120	115

600	x=0	420	220(biggest)	440(biggest)
600	7.2×10^{19} (x=0.05)	245	215	248
600	2.6×10^{20}(x=0.25)	170	160	165
800	x=0	300	185(biggest)	345(biggest)
800	2.8×10^{20}(x=0.25)	180	150	178
1000	3.2×10^{20}(x=0.25)	175	146	180