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Two-Dimensional GaGeTe Film: A Promising Graphene-Like Material with Tunable Band Structure and High Carrier Mobility

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Table S1 The optimized lattice constants (*a*), bond length for Ge-Ge, Ge-Ga and Ga-Te, bond angle <Ge-Ge-Ge , buckling height h_{Ge-Ge} , band gap withand without SOC in GaGeTe films respectively.

Layers	*a* (Å)	d(Ge-Ge)	d(Ge-Ga)	d(Ga-Te)	<Ge-Ge-Ge	h_{Ge-Ge}	Gap (w/o SOC)	Gap(w/SOC)
1N	4.153	2.524	2.485	2.709	110.35	0.0248	0.743	0.745
2N	4.134	2.521	2.478	2.694	110.07	0.0191	0.656	0.544
3N	4.131	2.519	2.474	2.691	110.07	0.0152	0.513	0.466
4N	4.126	2.514	2.471	2.682	110.08	0.0101	0.338	0.388
5N	4.123	2.509	2.468	2.680	110.12	0.0092	0.217	0.213
6N	4.114	2.507	2.463	2.676	110.12	0.0087	0.153	0.124

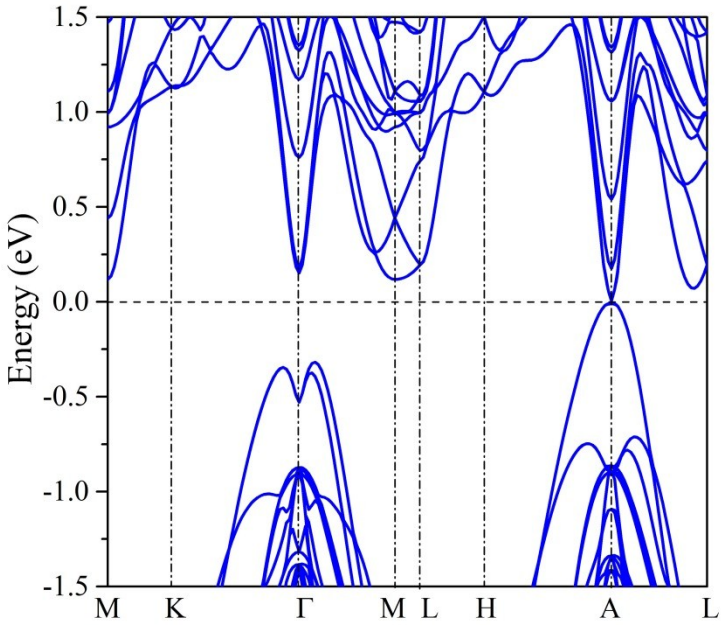

Figure S1 The calculated band structure of 3D bulk GaGeTe crystal. It shows a semimetal nature with a zero density of states at A point, in analogy to pristine germanene.

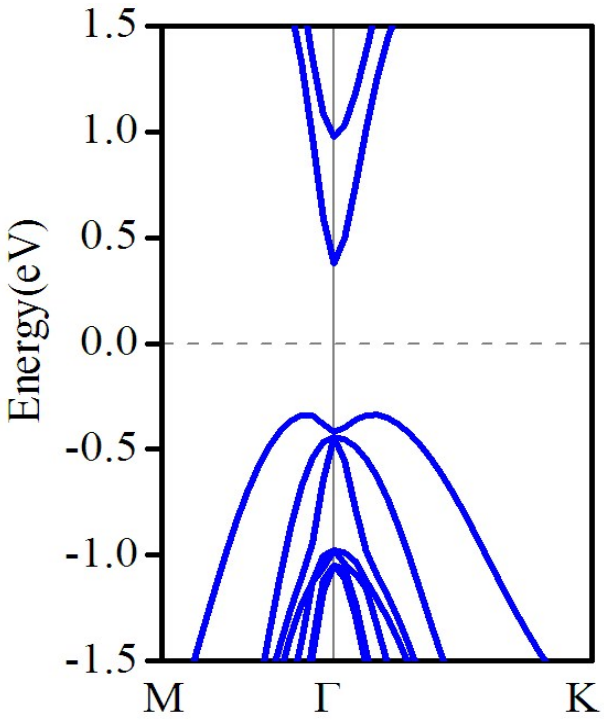

Figure S2 The calculated band structure of GaGeTe monolayer with the inclusion of SOC. Obviously, there is only a light influence on the band structure in particular concerning band gap when considering the effect of SOC.