

Supplementary information

Adsorption energy per adatom for the CGT-adatom system							
	11.11%	25%	33.33%	50%	66.66%	75%	100%
H	-0.23925	-0.81719	-0.81667	-1.38794	-0.81649912 4	-1.96255	-0.81617
Li	-2.44164	-2.43205	-2.42827172	-2.26267	-2.38432	-2.32015	-2.30730
Na	-1.96714	-1.92521	-1.90671	-1.84035	-1.79579	-1.71733	-1.69286
K	-2.30768	-2.23957	-2.19830	-2.04892	-1.99000	-1.93022	-1.81510
Rb	-2.31188	-2.24115	-2.19744	-2.05722	-1.96461	-1.90533	-1.78191
Ca	-2.69182	-2.59536	-2.58341	-2.72730	-3.25655	-3.10256	-2.22429

Table 1

TABLE. 1. The adsorption energy per adatom for the CGT-adatom system is shown the tables against different concentrations. On the x-axis the different concentrations is mentioned, while on the y-axis the adsorbed elements are shown.

Magnetic moment per unit cell of the CGT mono-layer							
U=2	11.11%	25%	33.33%	50%	66.66%	75%	100%
H	5.89	5.75	6.000	6.500	5.3334	6.7500	5000
Li	6.111	6.250	6.333	6.500	6.667	6.25	7.000
Na	6.111	6.250	6.334	6.500	6.667	6.75	7.000
K	6.111	6.250	6.333	6.500	6.667	6.750	7.000
Rb	6.111	6.250	6.333	6.500	6.667	6.750	7.000
Ca	6.222	6.500	6.667	7.000	6.667	7.000	7.100

Table 2

TABLE. 2. The magnetic moments of the CGT-adatom system for different concentrations are shown the tables. On the x-axis the different concentrations is mentioned. The elements are also shown for the corresponding adatoms.

Calculations based on PBE functional do not take into account the energy associated with the coulomb repulsion among the localized *d*- or *f*-orbital electrons. We include the Hubbard U parameter (i.e. PBE+U) in order to consider the contribution of the on-site coulomb interactions. However, it is very important to choose suitable value regarding the hubbard U value for a particular system. The Cr₂Ge₂Te₆ (CGT) possess Cr element which has localized *d*-orbital. Therefore, we tested different hubbard U values in order to find best U value for the 2D CGT system. As a result, we chose U=2eV since the FM order is more stable than AFM for this value as shown in the Fig S1(b).

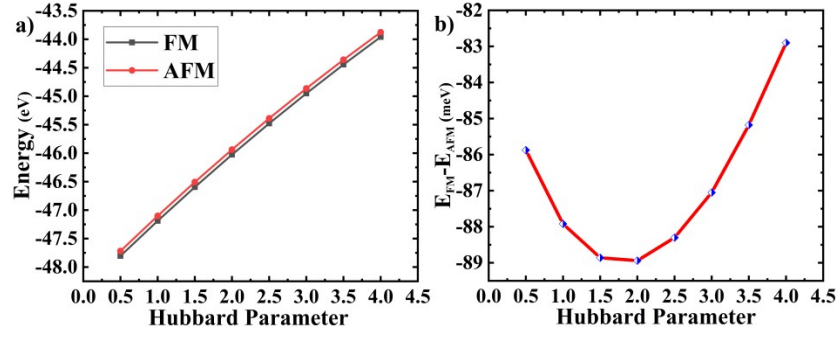


Fig. S1. (Color online) The FM, AFM, and $E_{FM} - E_{AFM}$ energies against different Hubbard U parameters are shown in a) and b) respectively.

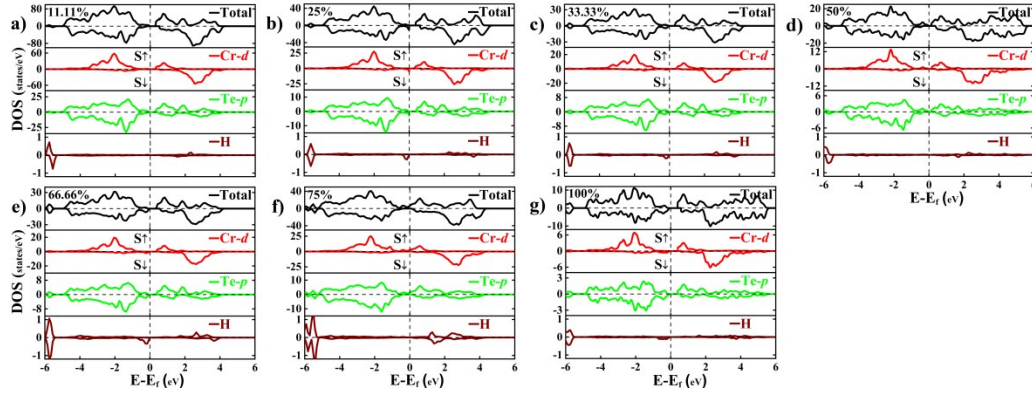


Fig. S2. (Color online) Spin-polarized electronic PDOS of CGT-H systems are depicted with different concentrations of the adatoms. The contribution of the orbitals is shown with different colors. The concentrations of the adatoms are mentioned in the corresponding plots.

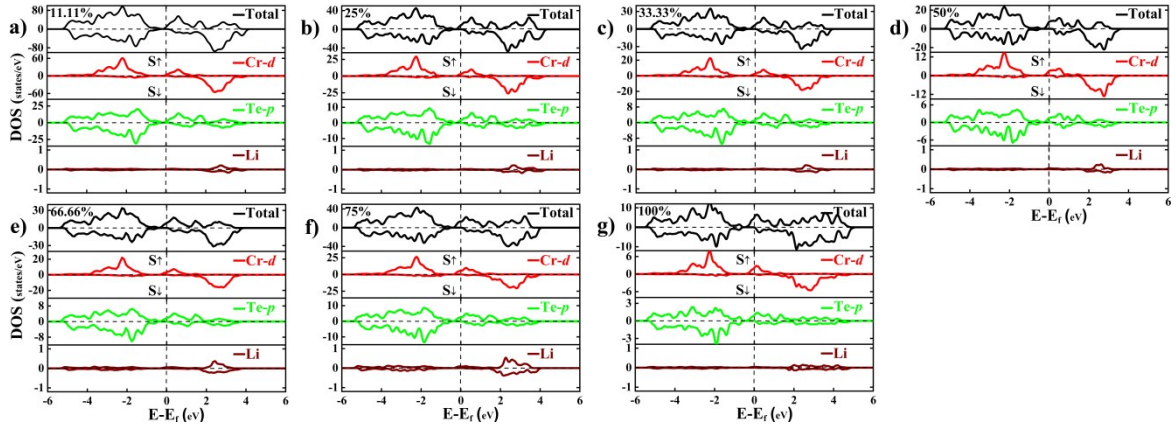


Fig. S2. (Color online) Spin-polarized electronic PDOS of CGT-Li systems are depicted with different concentrations of the adatoms. The contribution of the orbitals is shown with different colors. The concentrations of the adatoms are mentioned in the corresponding plots.

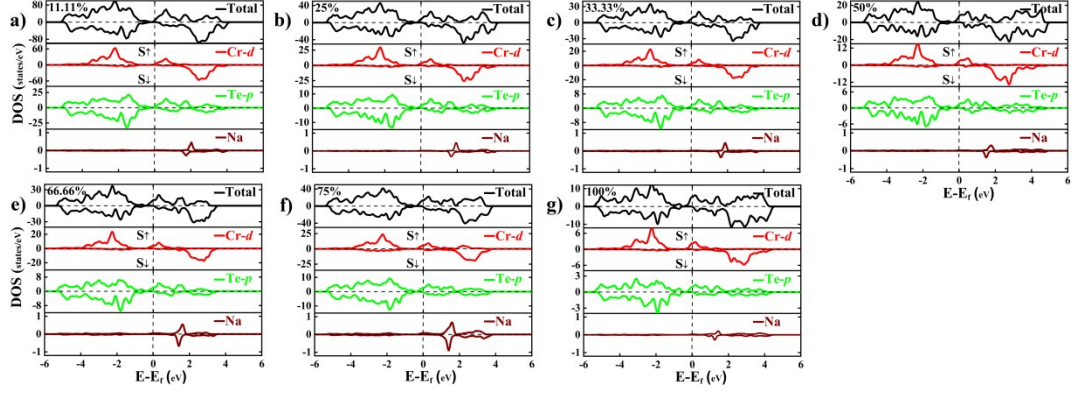


Fig. S4. (Color online) Spin-polarized electronic PDOS of CGT-Na systems are depicted with different t concentrations of the adatoms. The contribution of the orbitals is shown with different colors. The concentrations of the adatoms are mentioned in the corresponding plots.

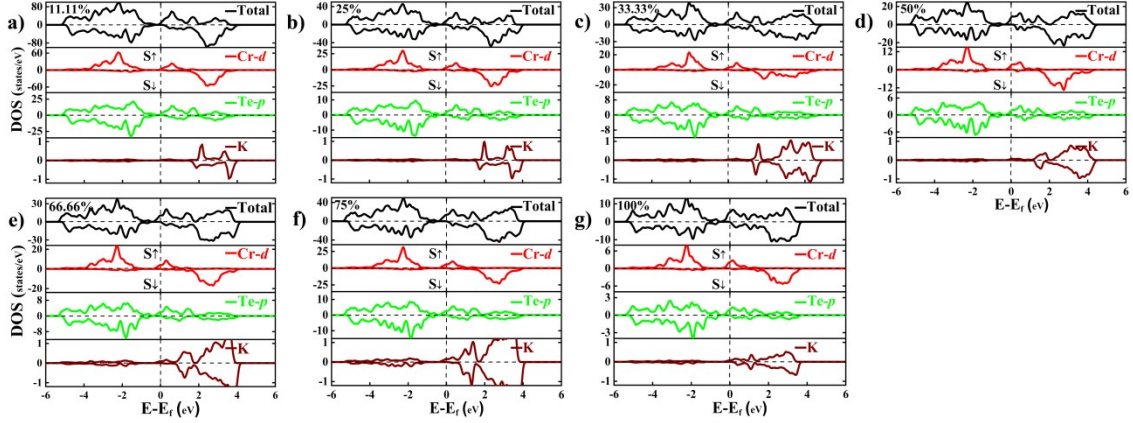


Fig. S5. (Color online) Spin-polarized PDOS of CGT-K systems are depicted with different t concentrations of the adatoms. The contribution of the orbitals is shown with different colors. The concentrations of the adatoms are mentioned in the corresponding plots.

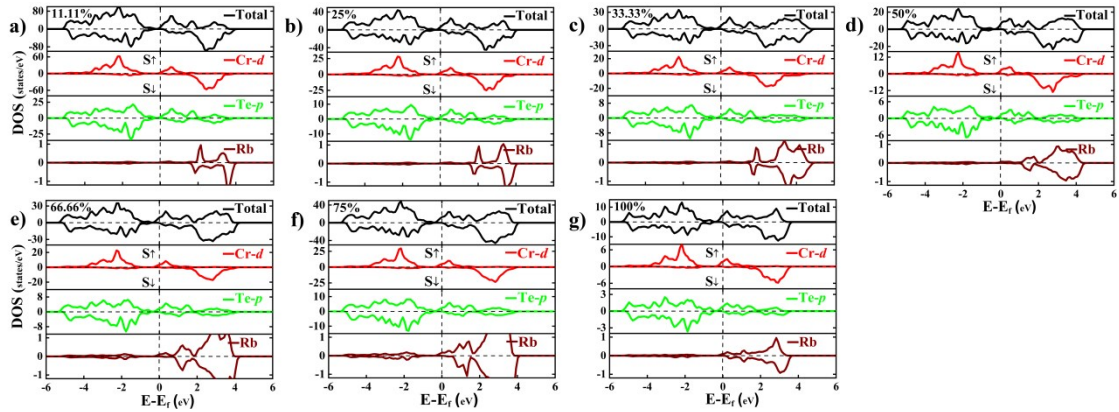


Fig. S6. (Color online) Spin-polarized electronic PDOS of CGT-Rb systems are depicted with different concentrations of the adatoms. The contribution of the orbitals is shown with different colors. The concentrations of the adatoms are mentioned in the corresponding plots.

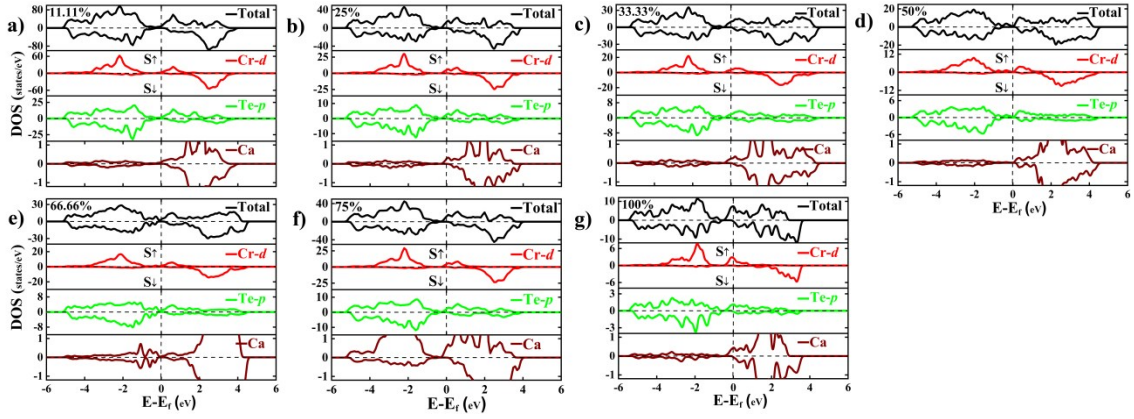


Fig. S7. (Color online). Spin-polarized electronic PDOS of CGT/Ca systems are depicted with different concentrations of the adatoms. The contribution of the orbitals is shown with different colors. The concentrations of the adatoms are mentioned in the corresponding plots.