Theoretical investigation of magnetic and optical properties in transition metal doped GaTeCl monolayer

Pengxia Zhou,[#*a] Ziheng Pan,[#a] Qian Gao,[a] Qian Zou,[a] Jieru Sun,[a] Yinxin Li,[a] You Qian,[a] Shang Li,[a] Chonggui Zhong,[*a,b] Lihua Qu,[a] Zhengchao Dong.[a]

[a]School of science, Nantong University, 226007

[b]School of Physical Science and Technology, Soochow University, Suzhou, 215006

[#]these authors contributed equally to this work.

*Corresponding author. Email: ntzhoupx@ntu.edu.cn or chgzhong@ntu.edu.cn

Supplementary Materials

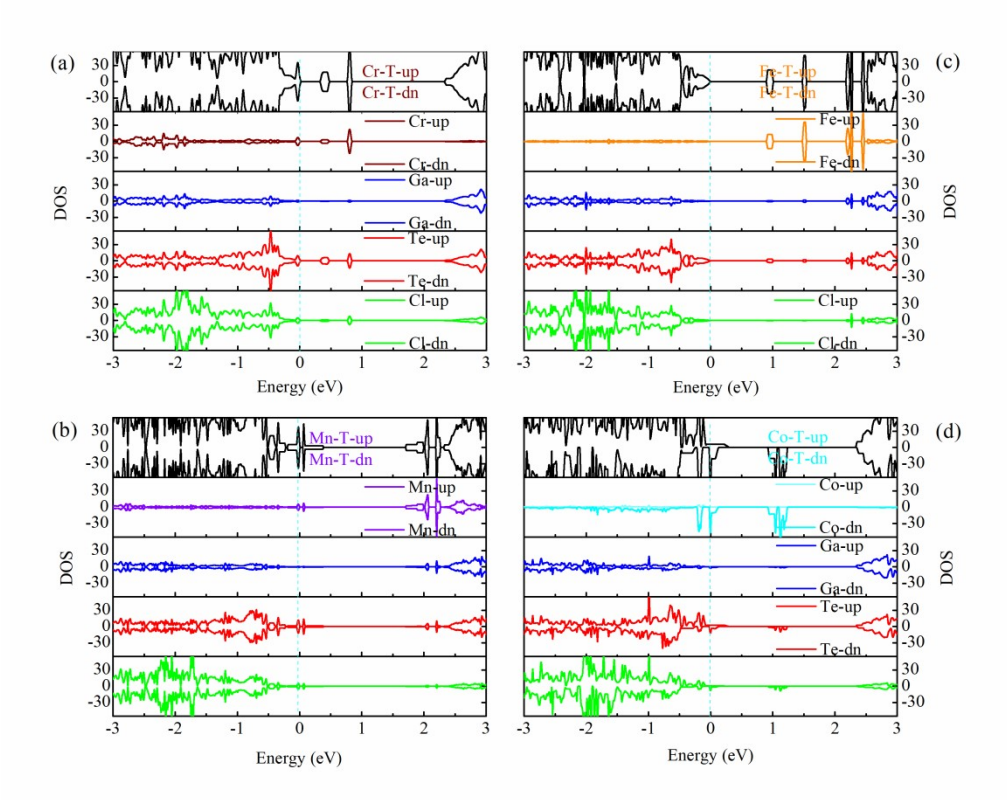

Fig. S1. (Color online) The total density of states (DOS) and projected DOS (PDOS) of (a) C-AFM Cr@GaTeCl, (b) A-AFM Mn@GaTeCl, (c) C-AFM Fe@GaTeCl, (d) FM Co@GaTeCl. Here, 0 eV denotes the Fermi energy, M-T-up (or dn) represent those total DOS of M@GaTeCl, the positive and negative of DOS correspond to the up spin state and down spin state respectively.

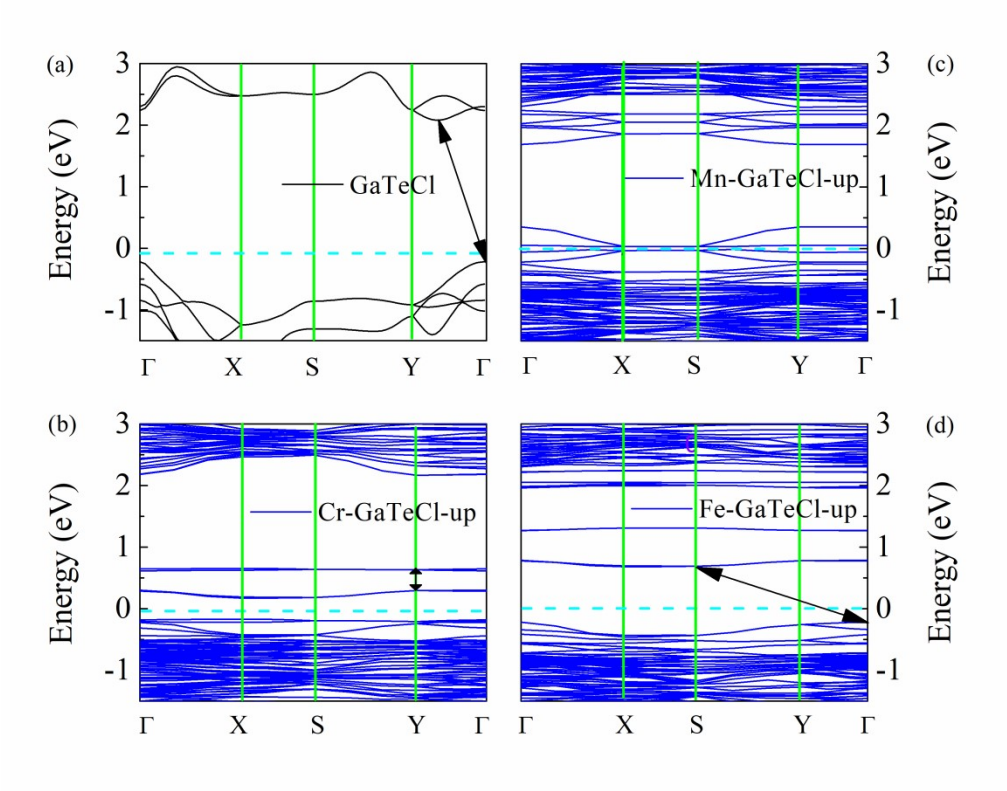

Fig. S2. (Color online) Band structures of GaTeCl and M@GaTeCl (M= Cr, Mn and Fe), (a) GaTeCl monolayer, (b) spin up Cr@GaTeCl, (c) spin up Mn@GaTeCl, (d) spin up Fe@GaTeCl. The black double arrow line denotes the K points of CBM and VBM of the system. For Mn@GaTeCl the K points of CBM and VBM are located between Γ and X points near Fermi energy. Due to that the spin up band structure is the same to the spin down one in the AFM M@GaTeCl systems (M = Cr, Mn, Fe and V), here, we only show the spin up band structure.