Supplement Materials

The role of group III, IV elements in Nb$_4$AC$_3$ MAX phases (A=Al, Si, Ga, Ge) and the unusual anisotropic behavior of electronic and optical properties

Fu Yu-dong$^a$, Baochang Wang$^{b,c}$, Yue Teng$^d$, Zhu Xiao-shuo$^a$, Feng Xiao-xue$^a$, Yan Mu-fu$^c$, Pavel Korzhavyi$^{d,e}$, Weiwei Sun$^{a,*}$

$^a$School of Material Science and Chemical Engineering & Key Laboratory of Superlight Materials and Surface Technology, Ministry of Education, Harbin Engineering University, Harbin 150001, China

$^b$Department of Physics and the Competence Centre for Catalysis, Chalmers University of Technology, 41296, Sweden

$^c$School of Material Science and Engineering, Harbin Institute of Technology, Harbin 150001, China

$^d$Department of Material Science and Engineering, KTH-Royal Institute Technology, Stockholm, SE-10044, Sweden

$^e$Institute of Metal Physics, Ural Division of the Russian Academy of Sciences, 620219 Ekaterinburg, Russia

In Fig. S1, it can be seen that the band structure of Nb$_4$GaC$_3$ and Nb$_4$AlC$_3$ are quite similar as Al and Ga have the same number of valence electrons. Similarly, the band structure of Nb$_4$SiC$_3$ and Nb$_4$GeC$_3$ also show similar features. Compared with Nb$_4$GaC$_3$ and Nb$_4$AlC$_3$, Nb$_4$GeC$_3$ and Nb$_4$SiC$_3$ have more bands across the Fermi level, indicating more states available for intra-band absorption in these two systems, especially for Nb$_4$SiC$_3$, which can be further verified by the calculated real part of the dielectric function. The Nb$_4$GaC$_3$ has more bands around Fermi level than Nb$_4$AlC$_3$ as well.
Fig. S1. The band structure of Nb$_4$AlC$_3$ (a), Nb$_4$SiC$_3$ (b), Nb$_4$GaC$_3$ (c), and Nb$_4$GeC$_3$ (d). The Fermi level is set to be 0 eV.