Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.
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Supplement Materials

The role of group III, IV elements in Nb_4AC_3 MAX phases (A=Al, Si, Ga, Ge) and the unusual anisotropic behavior of electronic and optical properties

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In Fig. S1, it can be seen that the band structure of Nb_4GaC_3 and Nb_4AlC_3 are quite similar as Al and Ga have the same number of valence electrons. Similarly, the band structure of Nb_4SiC_3 and Nb_4GeC_3 also show similar features. Compared with Nb_4GaC_3 and Nb_4AlC_3, Nb_4GeC_3 and Nb_4SiC_3 have more bands across the Fermi level, indicating more states available for intra-band absorption in these two systems, especially for Nb_4SiC_3, which can be further verified by the calculated real part of the dielectric function. The Nb_4GaC_3 has more bands around Fermi level than Nb_4AlC_3 as well.

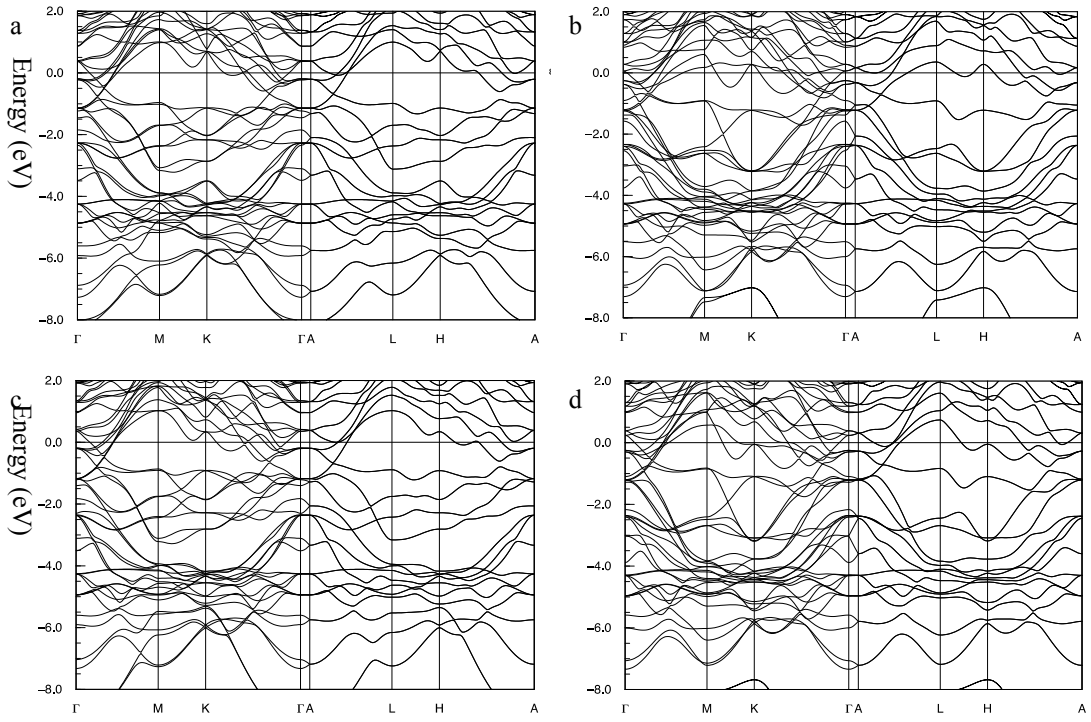

Fig. S1. The band structure of Nb_4AlC_3 (a), Nb_4SiC_3 (b), Nb_4GaC_3 (C), and Nb_4GeC_3 (d). The Fermi level is set to be 0 eV.