Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information for

Exploration of New Ferromagnetic, Semiconducting and Biocompatible Nb_3X_8 (X=Cl, Br or I) Monolayers with Considerable Visible and Infrared Light Absorption

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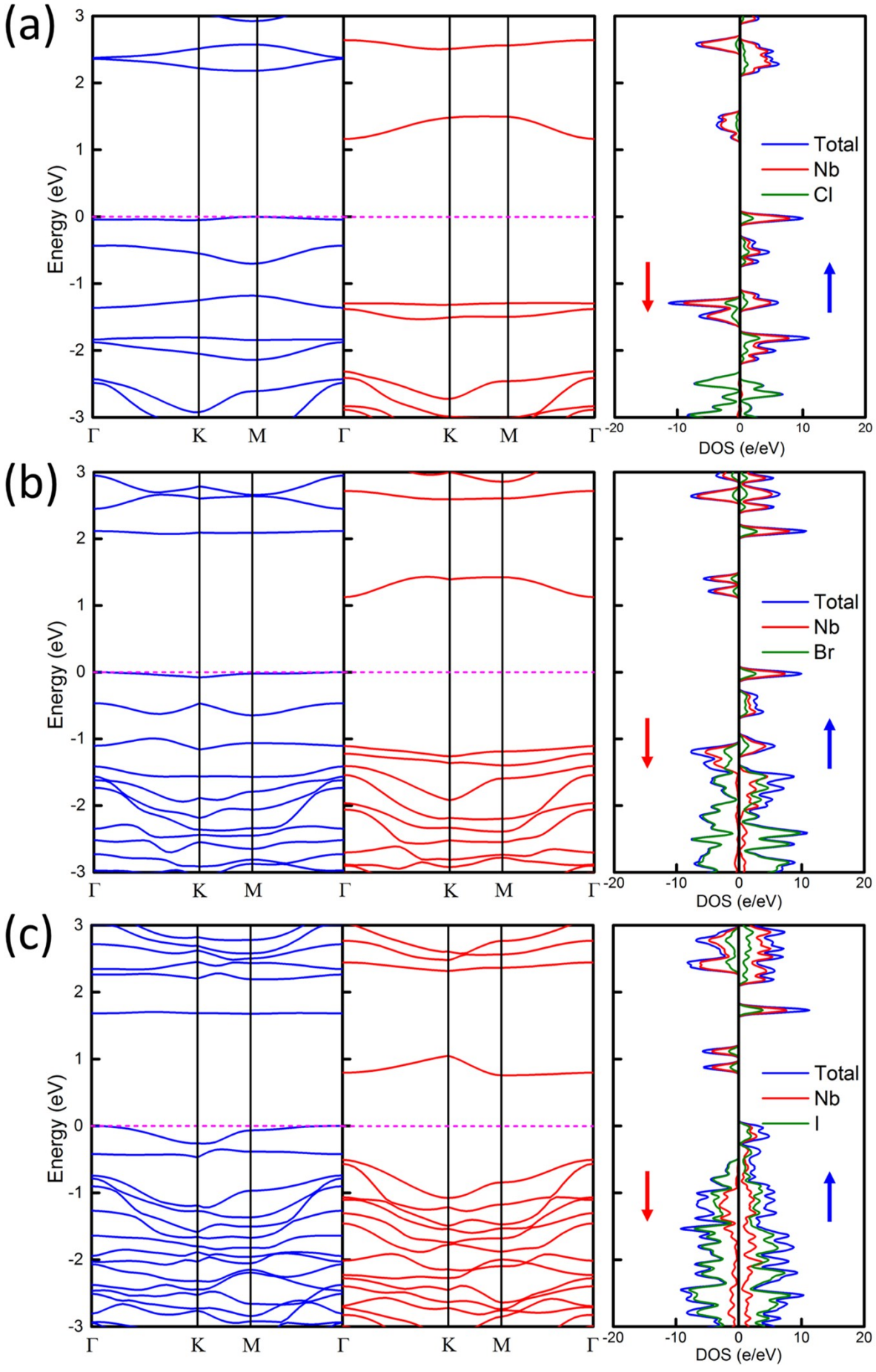

Fig. S1. Band structure and corresponding density of states of (a) Nb_3Cl_8, (b) Nb_3Br_8 and (c) Nb_3I_8 monolayers calculated in HSE06 theoretical level, respectively.

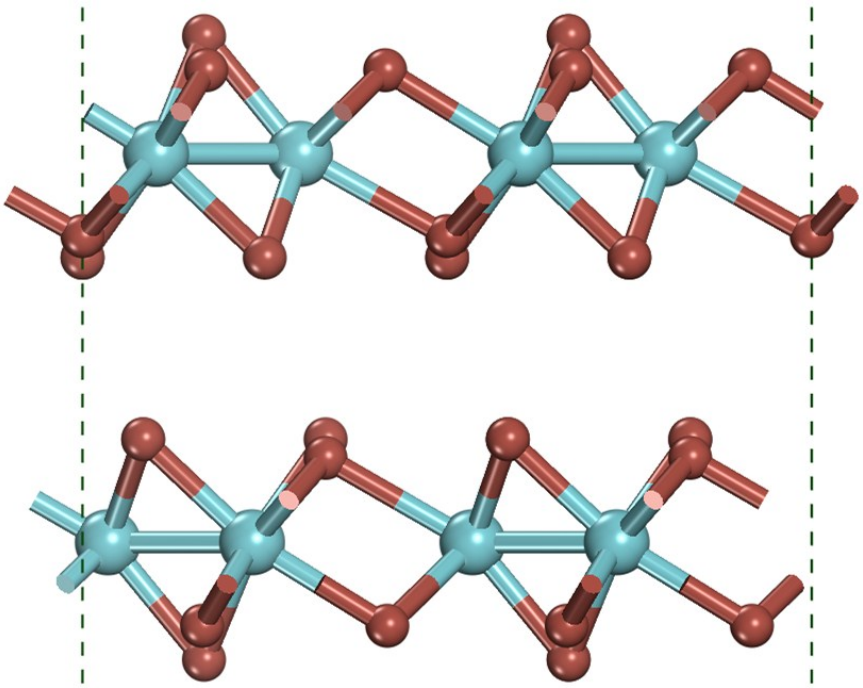

Fig. S2. Side view of optimized geometries of Nb_3I_8 bilayer.

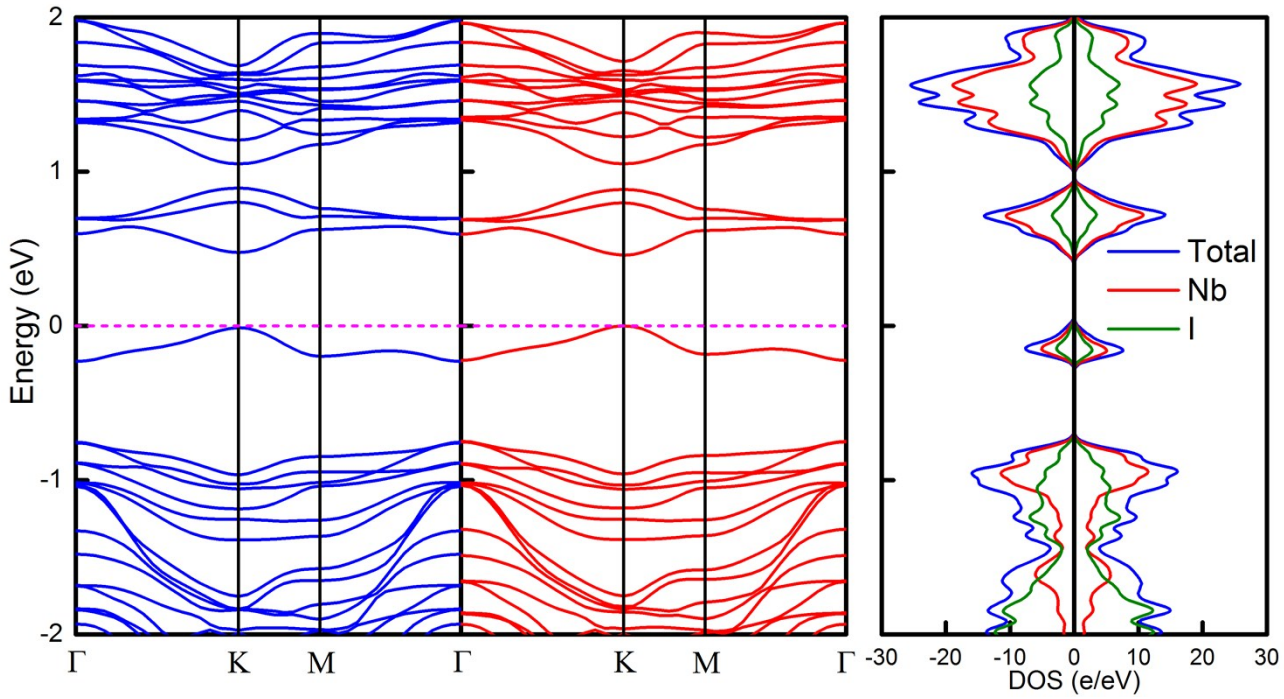

Fig. S3. Band structure and corresponding density of states of Nb_3I_8 bilayer.

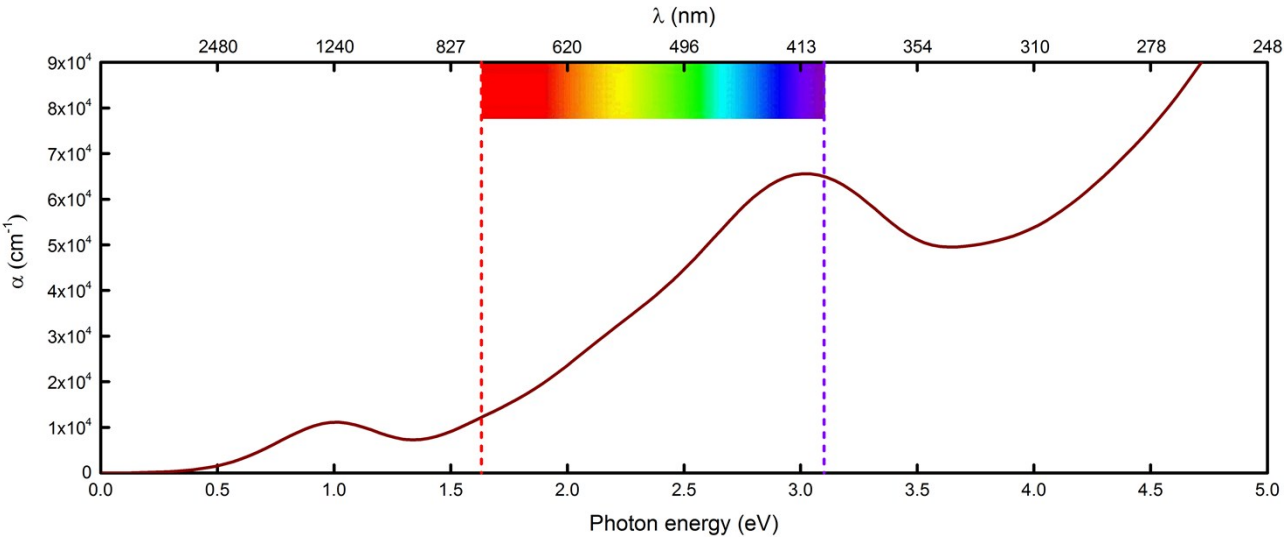

Fig. S4 Optical absorption coefficients α for Nb_3I_8 bilayer. The seven-colour-light area between the red and the purple lines represents the visible light range.