Supporting Information

for

Novel Titanium Nitride Halides TiNX (X = F, Cl, Br) Monolayers: Potential Materials for High Efficient Excitonic Solar Cells

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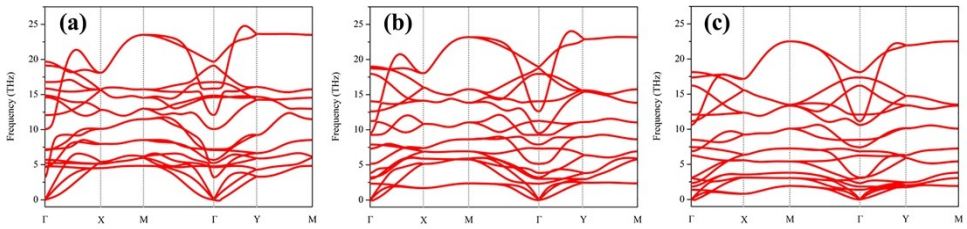

Fig. S1 The phonon dispersion curves of monolayer (a) TiNF, (b) TiNBr and (c) TiNI.

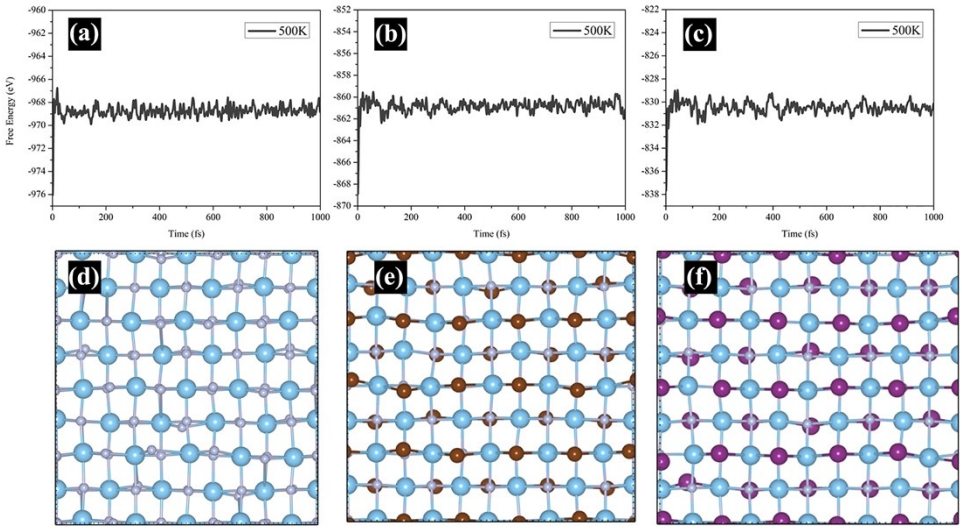

Fig. S2 Variation of total energys at 1 ps during *ab initio* MD simulation at temperature of 500K and top views of snapshot at 1 ps of the *ab initio* MD simulation for monolayer TiNF (a)(d), TiNBr (b)(e) and TiNI (c)(f).

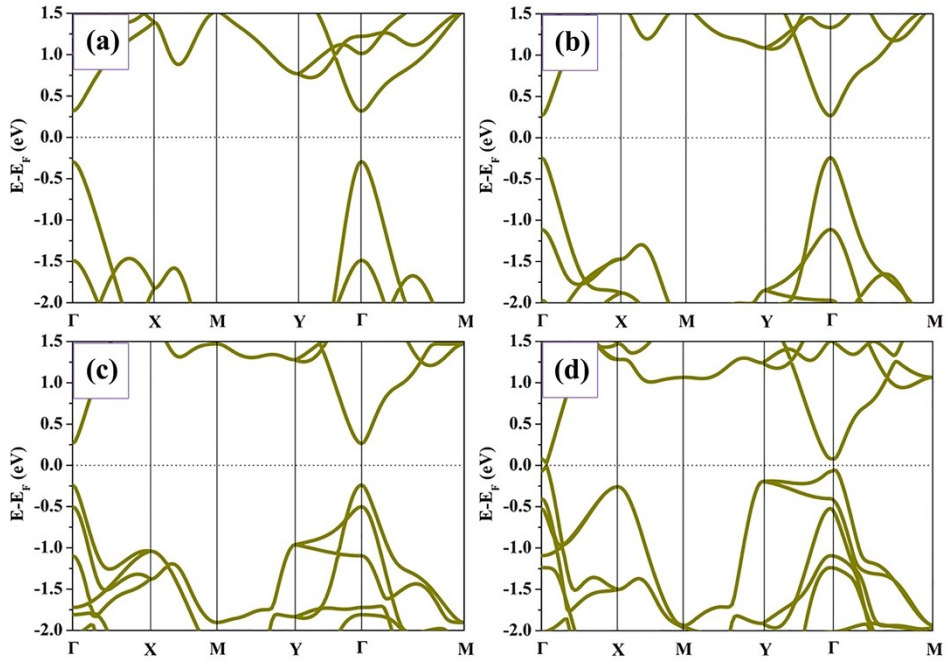

Fig. S3 PBE band structures of (a) TiNF, (b) TiNCl, (b) TiNBr and (d) TiNI monolayers. The dashed line denotes the Fermi energy.

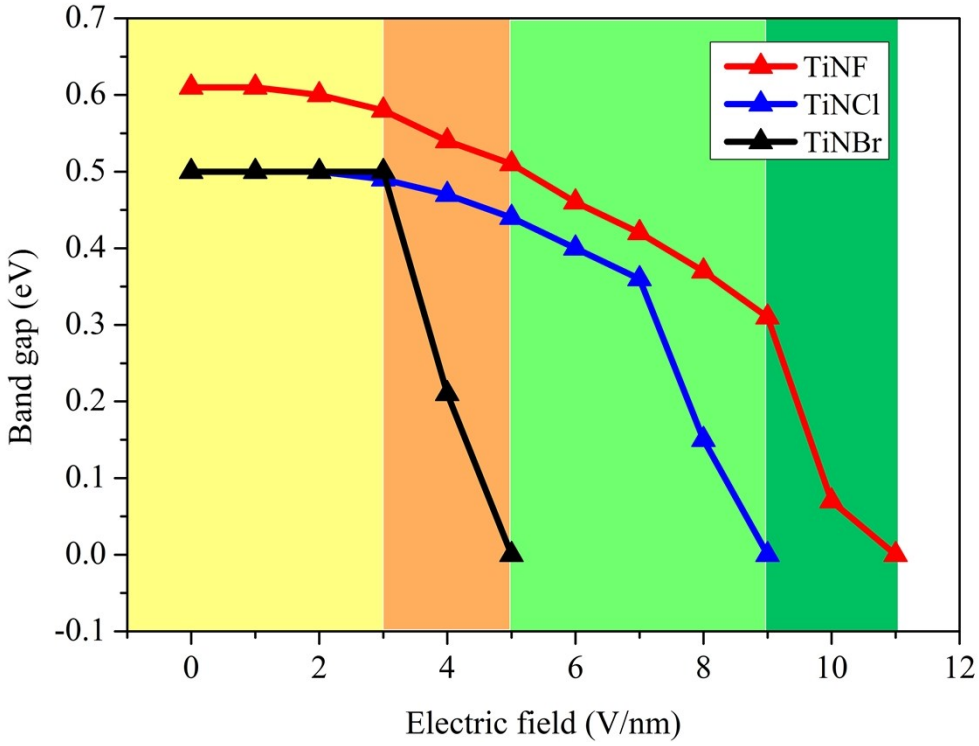

Fig. S4 The electronic band gap of TiNX (X = F, Cl ,Br) under a perpendicular electric field that along z direction.

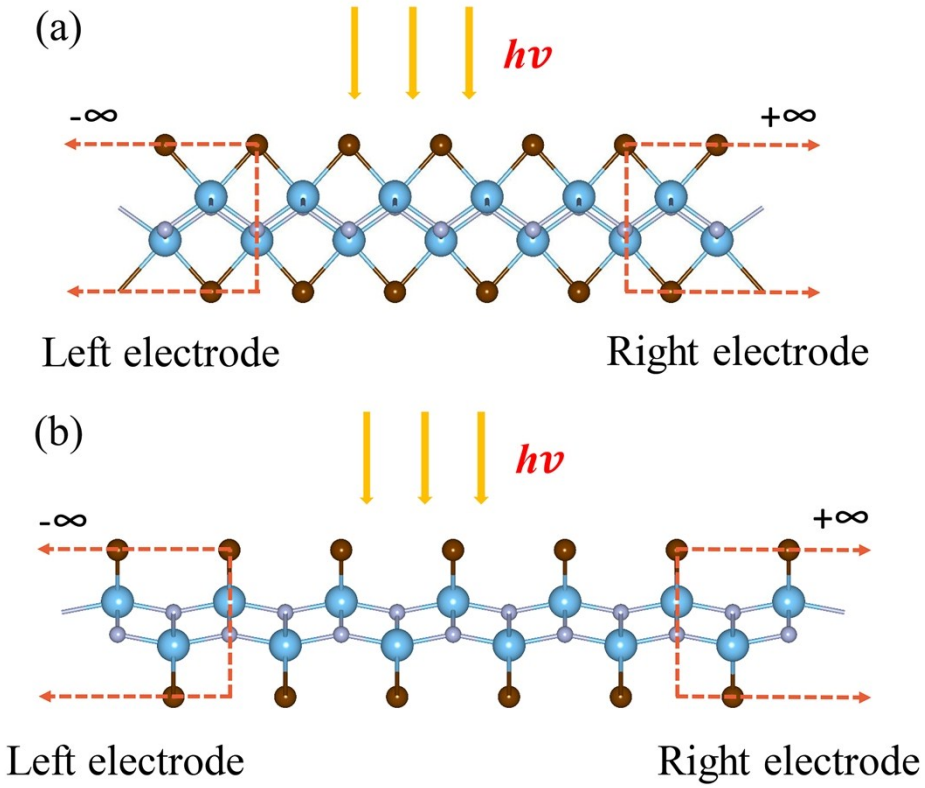

Fig. S5 Schematics of the two-probe device models for calculating the photocurrent of TiNX monolayers along (a) x and (b) y directions.

As shown in Fig. S5, two-probe models are adopted, which are constructed with a center scattering region and two semi-infinite TiNX sheets electrodes. Due to the absent of asymmetry in both directions, we applied 0.2 V external bias voltage across the scattering region along x or y directions. The generated electron-hole pairs are swept to electrodes in different directions because of the drain-souce electric field, leading to the photoinduced current.

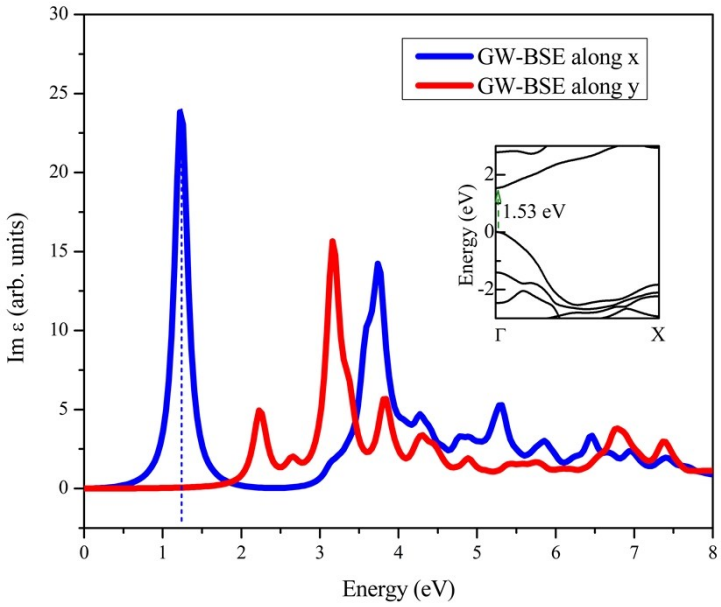

Fig. S6 Optical spectra of TiNBr monolayer calculated using GW-BSE method for linearly polarized light along x direction and y direction. The inset represents the electronic structure of TiNBr monolayer calculated by GW method.

Our calculation shows that the first absorption peak is located at 1.22 eV, below the direct G_0W_0 gap of 1.53 eV, which is a weakly bounded excitonic state with binding energy of 0.31 eV.