Supporting Information
Influence of chalcogen composition on the structural transition and on the electronic and optical properties of the monolayer titanium trichalcogenide ordered alloys

F. Ersan,¹ H. Duygu Ozaydin,¹ and E. Aktürk¹,²,*
¹Department of Physics, Adnan Menderes University, Aydın 09010, Turkey
²Nanotechnology Application and Research Center, Adnan Menderes University, Aydın 09010, Turkey
(Dated: December 14, 2017)

PACS numbers: 62.23.Kn, 71.15.Mb, 73.22.-f, 71.20.-b

I. OPTICAL PROPERTIES

From the dynamical dielectric response functions ε(ω), absorption coefficient α(ω) can be obtained. We calculated it by using the following equation:

\[ \alpha(\omega) = \sqrt{2} \omega \left[ \sqrt{\varepsilon_1(\omega)^2 + \varepsilon_2(\omega)^2} - \varepsilon_1(\omega) \right]^{1/2} \]  

* Electronic address: ethem.akturk@adu.edu.tr
FIG. 1: (Color online) Considered of all possible TiX$_3$(1−x)X$_x$ monolayers as a function of the chalcogen atoms concentration $x$. TiS$_{3(1−x)}$Se$_{3x}$ alloys are illustrated for instance.
FIG. 2: (Color online) Lattice constants of TiX$_{3(1-x)}$X$_x$ monolayers along a- and b- directions as a function of the chalcogen atoms concentration $x$ for all considered possible structures.
FIG. 3: (Color online) Electronic band structure of TiS$_{3(1-x)}$Se$_{3x}$ monolayers for the energetically most favorable structural allotropes with HSE methods.
FIG. 4: (Color online) Absorption spectrum of energetically favorable TiS$_{(3\gamma)}$Se$_{3\gamma}$ monolayers as a function of photon energy for different concentration.