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

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I. OPTICAL PROPERTIES

From the dynamical dielectric response functions $\varepsilon(\omega)$, absorption coefficient $\alpha(\omega)$ can be obtained. We calculated it by using the following equation;

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

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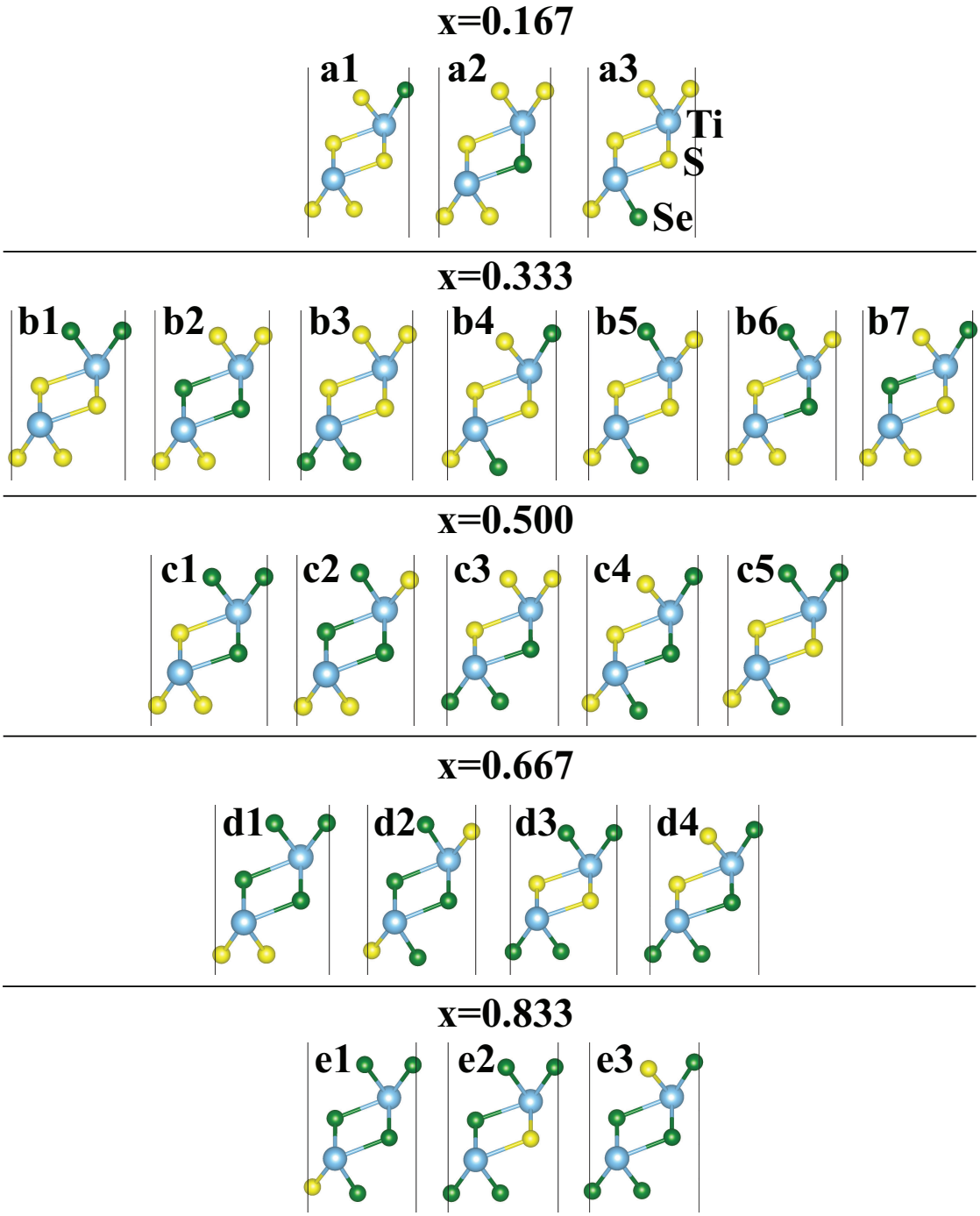

FIG. 1: (Color online) Considered of all possible $TiX_{3(1-x)}X'_{3x}$ monolayers as a function of the chalcogen atoms concentration x. $TiS_{3(1-x)}Se_{3x}$ alloys are illustrated for instance.

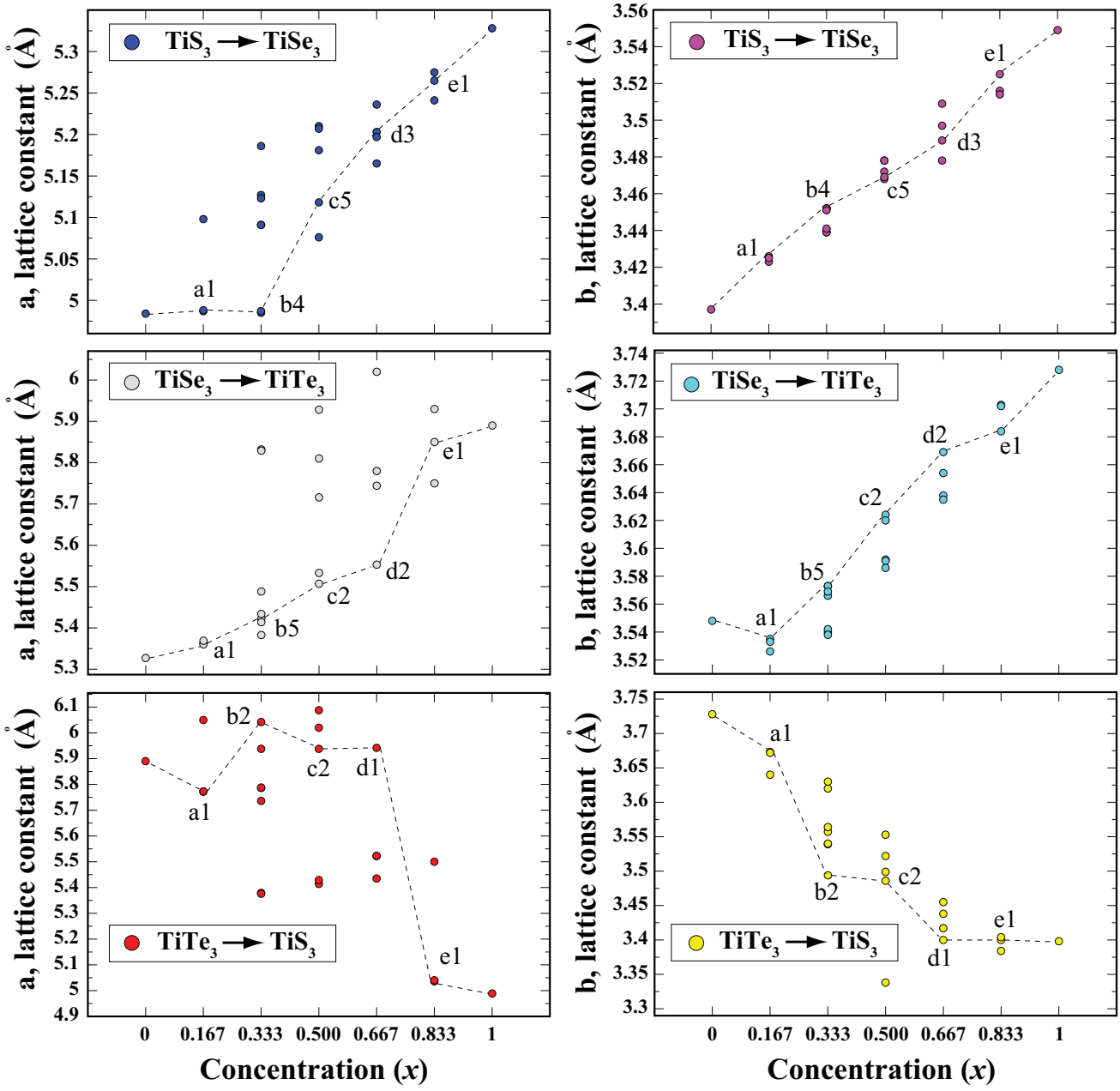

FIG. 2: (Color online) Lattice constants of $TiX_{3(1-x)}$ X'_{3x} monolayers along a- and b- directions as a function of the chalcogen atoms concentration x for all considered possible structures.

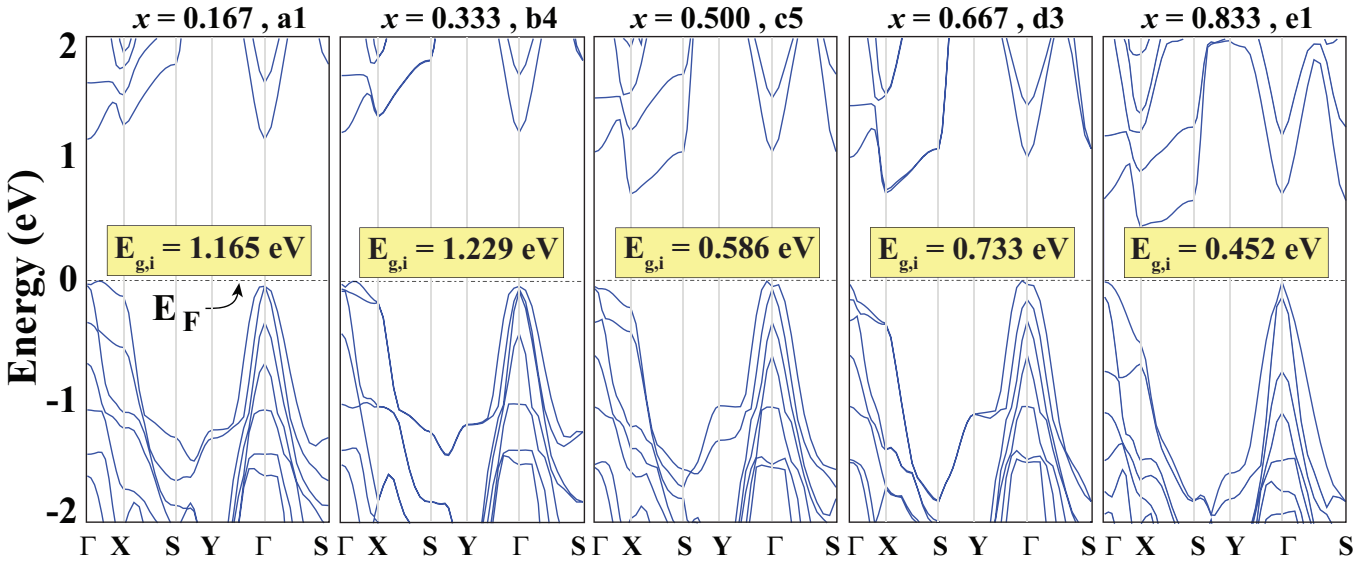

FIG. 3: (Color online) Electronic band structure of $TiS_{3(1-x)}Se_{3x}$ monolayers for the energetically most favorable structural allotropes with HSE methods.

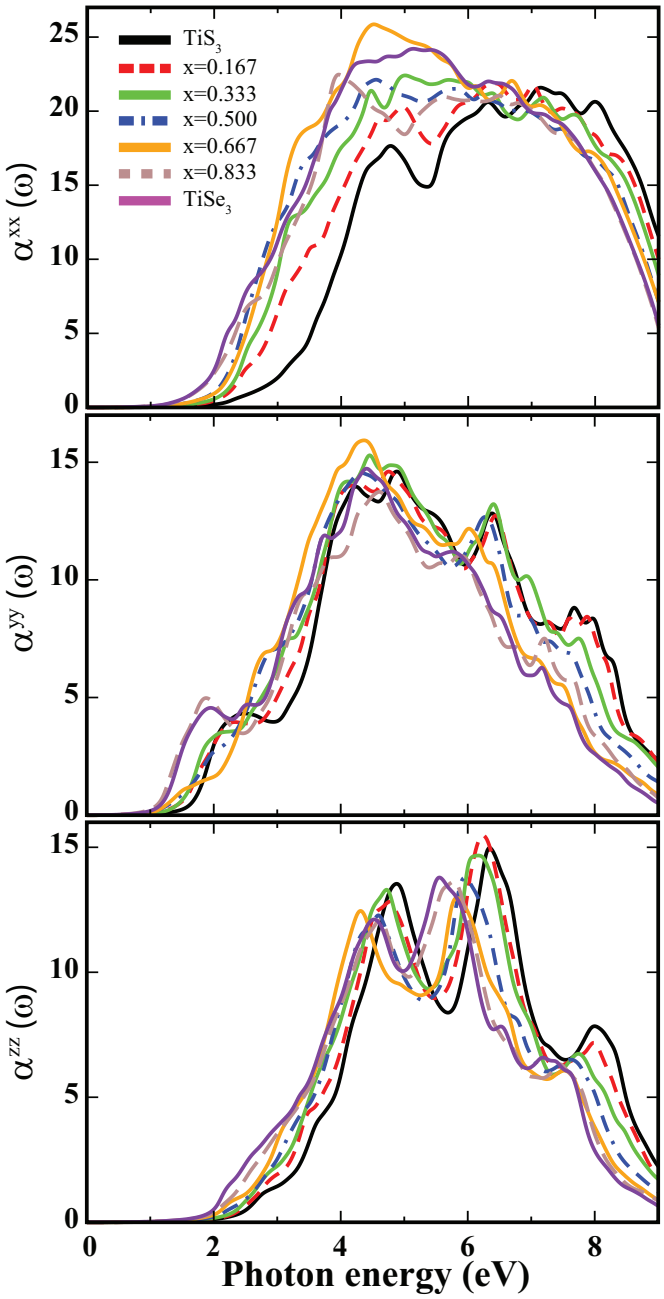

FIG. 4: (Color online) Absorption spectrum of energetically favorable $TiS_{3(1-x)}Se_{3x}$ monolayers as a function of photon energy for different concentration.