Supplementary Information

Two-dimensional antimonene as a potential candidate for dioxin capture

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SI Further analysis for the MD simulations

Further analysis has been performed for the MD simulations. Specifically, we calculated the Ti-O and Sb-O distances in the Ti-TCDD and Sb-TCDD complexes, respectively, throughout the trajectory. These results are displayed in Figure S1(a). Our observations revealed that these distances exhibited fluctuations around their optimal values in the optimized structures during the entire MD run. This dynamic behavior suggests that TCDD remains firmly adhered to the surface, providing compelling evidence for the stability of these complexes. Additionally, we employed an alternative approach by calculating the distance solely in the z-direction between the COM of the TCDD molecule and the surface, see Figure S1(b). Consistently, these values fluctuated around their optimal counterparts in the optimized structures, further reinforcing the adherence of TCDD to the surface.

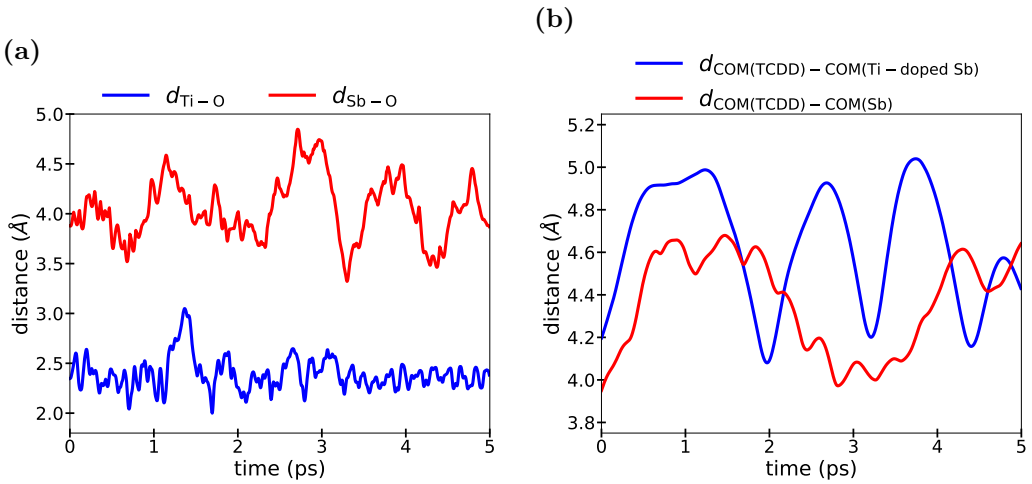

Figure S1: Time evolution of (a) Ti-O and Sb-O distances, and (b) the distances between the center of mass (COM) of the TCDD and the COM of the surface of antimonene (red) or Ti-doped antimonene (blue) in z direction.

SI.i Adsorption energy throughout the MD trajectories

For a more detailed analysis of the adsorption strengths, approximately 1000 snapshots were selected from a total of 10,000 steps captured at intervals of 0.005 ps during the MD simulation. Subsequently, the interaction energies between TCDD and the surface were computed according to Eq. 1, then corrected according to Eq. 2. Notably, the results consistently indicated negative

interaction energies in both cases, signifying the persistent adsorption of TCDD to the surface throughout the entire MD simulation. Furthermore, it was observed that the values of interaction energies fluctuated around the adsorption energy values calculated for the optimized structures in the stationary calculations discussed in the main manuscript (refer to the previous section, particularly Figure 4 and Table 3).

Moreover, an interesting observation emerged, highlighting a substantial difference between Sb-TCDD and Ti-TCDD. In Sb-TCDD, the fluctuation window of interaction energy ($\approx$ 0.3 eV) is significantly narrower compared to its counterpart in the case of Ti-TCDD ($\approx$ 3.0 eV). This discrepancy is attributed to the pronounced deformation of the TCDD structure when adsorbed on the Ti-doped antimonene surface. Consequently, in MD simulations, there is a higher degree of variation in the internal geometry of TCDD, resulting in instances of notably high or low interaction energies. Conversely, the adsorption of TCDD on pure antimonene does not induce such extensive deformation, allowing TCDD to maintain its planar structure. Consequently, during the MD simulation, the internal structure of TCDD undergoes minimal change. In summary, in the case of Ti-TCDD, the predominant dynamical behavior of TCDD pertains to internal structural vibrations, while in the case of Sb-TCDD, the primary dynamical behavior involves translation motion in the xy plane. For a better understanding of these dynamic behaviours, movies of the MD simulation were created and can be found in the supplementary information materials.

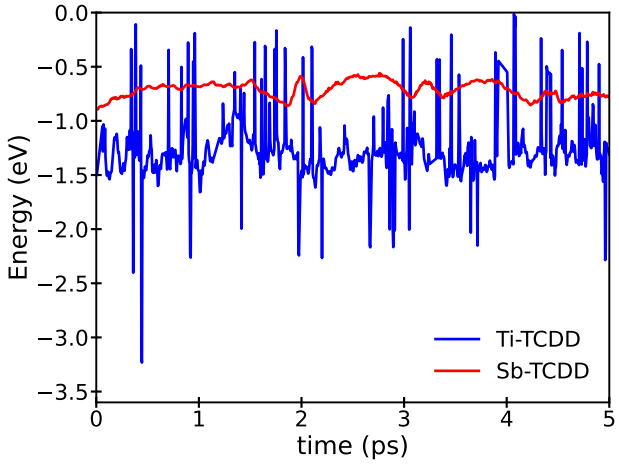

Figure S2: Interaction energies (calculated according to Eq. 1, then corrected according to Eq. 2) of selected snapshots ($\approx$ 1000 out of 10000 steps) throughout the MD trajectories.

SII DOS

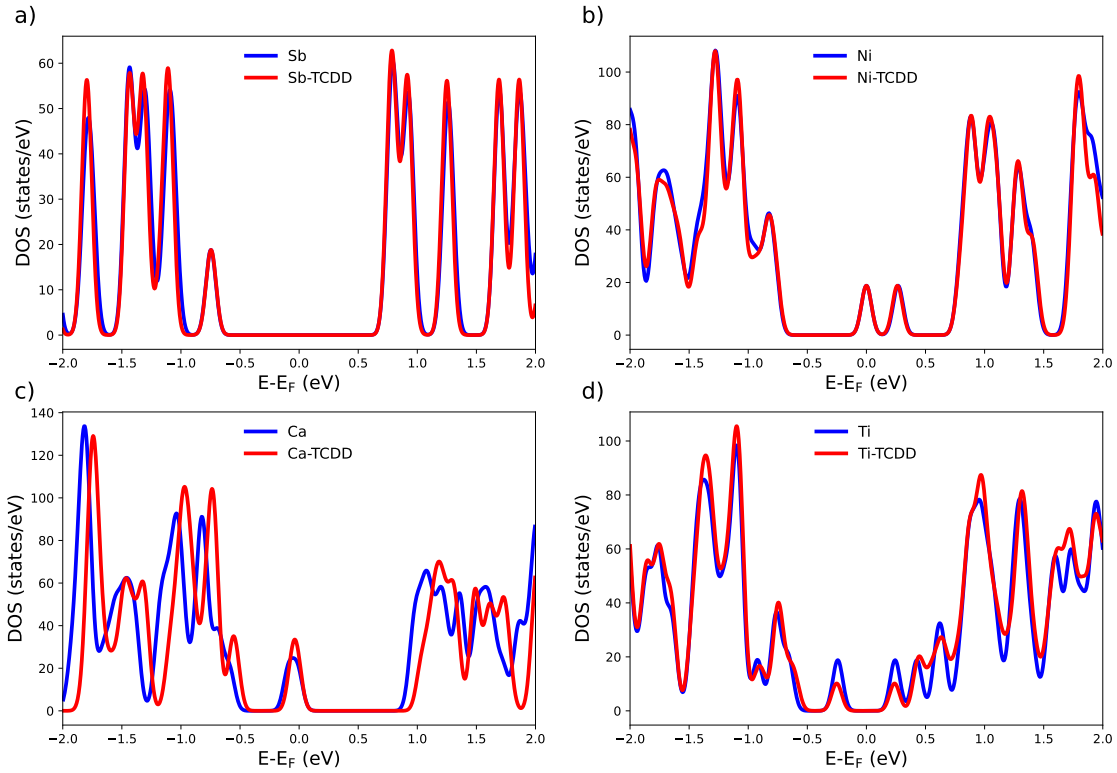

Figure S3: DOS of pristine and doped antimonene versus their corresponding complexes (only parallel configuration)

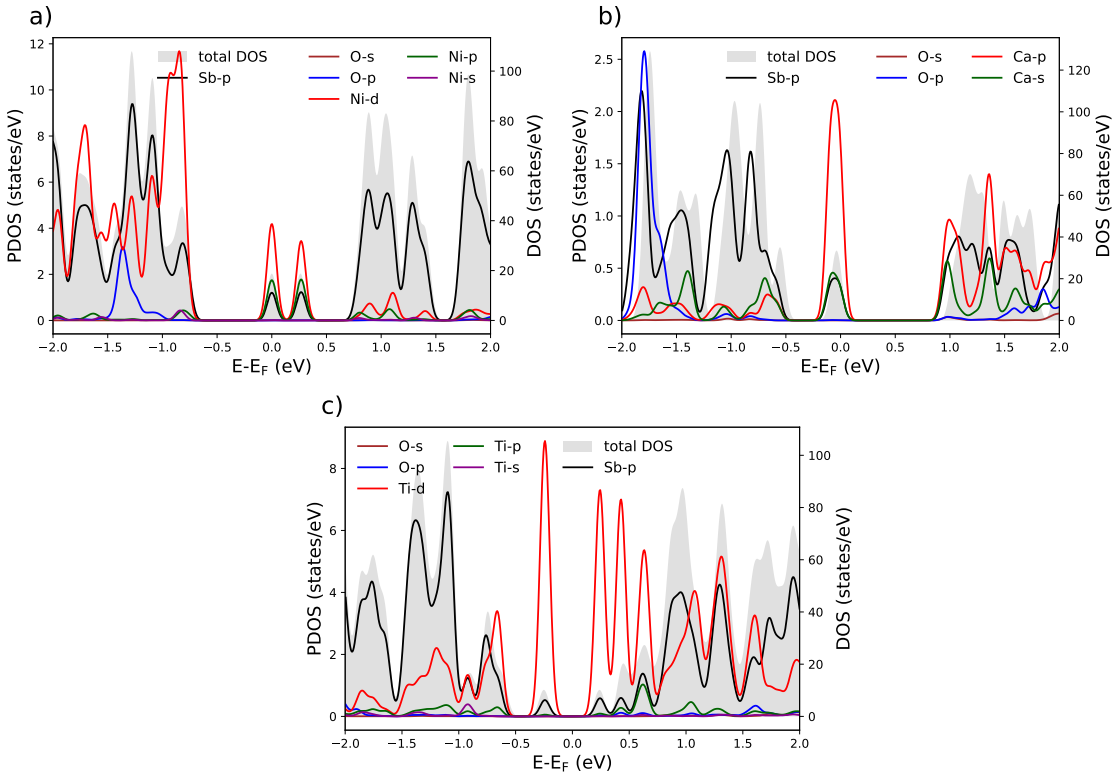

Figure S4: PDOS of oxygen (TCDD) and dopant atoms of the doped antimonene. Note that the black lines correspond to the contribution of Sb to the DOS. The corresponding total DOS for each system is shown in the background.