Supporting Information

The line defects in two-dimensional Bi_2O_2S: enhanced photocurrents in the infrared region

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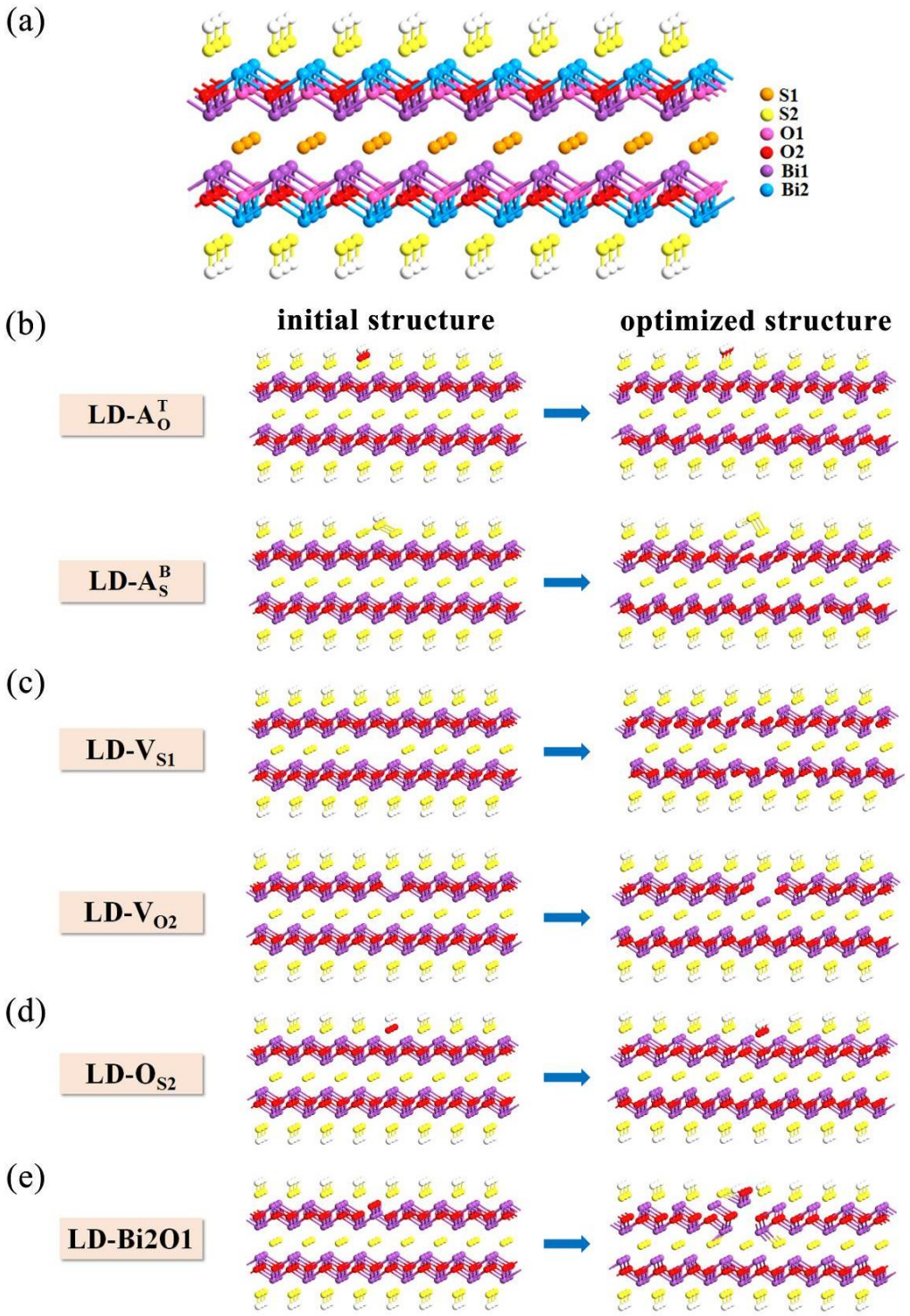

Fig. S1 (a) The perfect structure of 2D Bi_2O_2S. Different atoms of the same element are distinguished by using different colors. The examples of the initial and the optimized structures of the line defects (b) $LD-A_O^T$, $LD-A_S^B$, (c) LD-V_{S1}, LD-V_{O2}, (d) LD-O_{S2} and (e) LD-Bi2O1.

Since the structures of line defects are usually more complicated than those of point defects, the design method of the initial structures is important and exquisite. To optimize the design process, according to the structural symmetry of the perfect "zipper" 2D Bi_2O_2S, all the atoms of the same element are divided into two categories, *i.e.* Bi1 and Bi2, O1 and O2, S1 and S2, as shown in Fig. S1a. For example, S1 indicates that the S atom is at the inner position, while S2 indicates that the S atom is at the surface of the 2D structure. Here, we mainly considered four typical intrinsic line defects:

I. By directly adsorbing a column of X (X=Bi, O or S) atoms on the surface of 2D Bi_2O_2S, one can obtain different initial structures of this type of line defects. Considering the structural symmetry of the surface, we mainly tested the top (T) and bridge (B) sites. Generally speaking, these adsorption-type line defects can be named as $\mathrm{LD-A_X^{T/B}}$. For the notation, "LD" is the abbreviation of "line defect", and "A" indicates the line defect can be obtained by "adsorbing" a column of atoms on the T or B sites of the surface. The examples $\mathrm{LD-A_O^T}$ and $\mathrm{LD-A_S^B}$ are given in Fig. S1b. In addition, inserting a column of atoms at the inner positions of 2D Bi_2O_2S will lead to extremely unstable structure, thus we will not consider and discuss these cases.

II. Similarly, by directly deleting a column of X atoms, we can obtain various initial structures for this type of line defects. Such vacancy-type line defect can be viewed as a column of vacancies (V), thus can be named as LD-V_X. However, different from method I, the vacancy-type line defects may also appear at the inner positions of 2D Bi_2O_2S. Therefore, for this kind of line defects, both cases were carefully considered and the corresponding examples are shown in Fig. S1c.

III. By replacing a column of X atoms with a column of Y atoms, one can obtain the antisite-type line defect LD-Y_X. In other words, this type of line defects can be viewed as a column of antisite atoms. In Fig. S1d, such line defect is illustrated by the example LD-O_{S2}, that is, a column of S2 atoms is replaced by a column of O atoms.

IV. This type of line defects can be viewed as exchanging a column of X atoms and a column of Y atoms (LD-XY). Fig. S1e shows an example of the exchange-type line

defect (LD-Bi2O1); in the structure a column of Bi2 atoms is replaced by a column of O atoms and, at the same time, a column of O1 atoms is replaced by a column of Bi atoms (please note that LD-Bi2O1 has many different structures and we only considered the most stable one). In fact, such line defects are special situations of method III. Nevertheless, we believe that it is necessary to discuss them separately.

The above-mentioned four types of line defects are relatively simple, but they are basic and important, since a lot of more complicated line defects usually can be viewed as certain combinations of these line defects. Here we will mainly focus on these "simple, basic but important" line defects. Based on the four design methods, we can obtain a variety of initial structures of the line defects and then optimize them at DFT level. To our knowledge, there is no systematic or special nomenclature for the line defects in 2D materials. Nevertheless, we believe the notations and explanations mentioned above can be effectively used to distinguish these different line defects in 2D Bi_2O_2S.

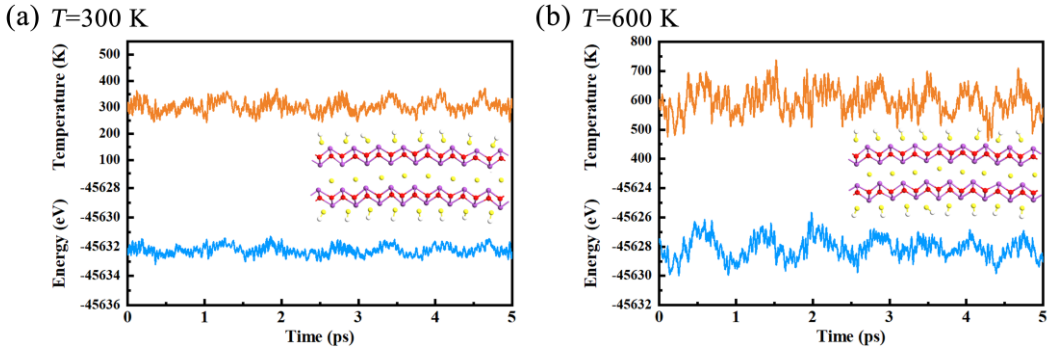

Fig. S2 The fluctuations of temperature and energy with time for 2D Bi_2O_2S at (a) 300 K and (b) 600 K. The inset shows the corresponding structure after 5000 time steps.

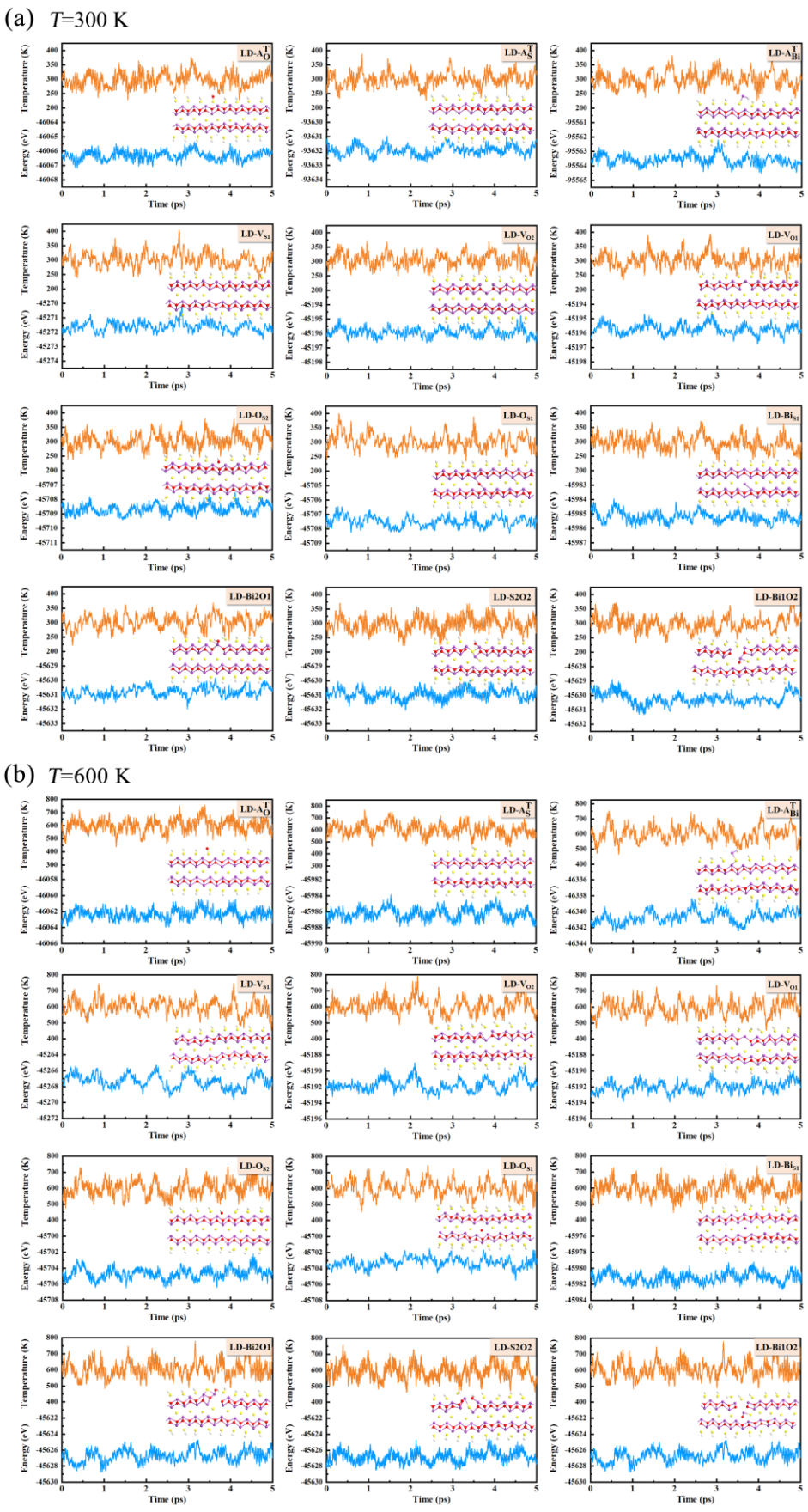

Fig. S3 The fluctuations of temperature and energy with time for adsorption-, vacancy-, antisite- and exchange-type line defects at (a) 300 K and (b) 600 K.

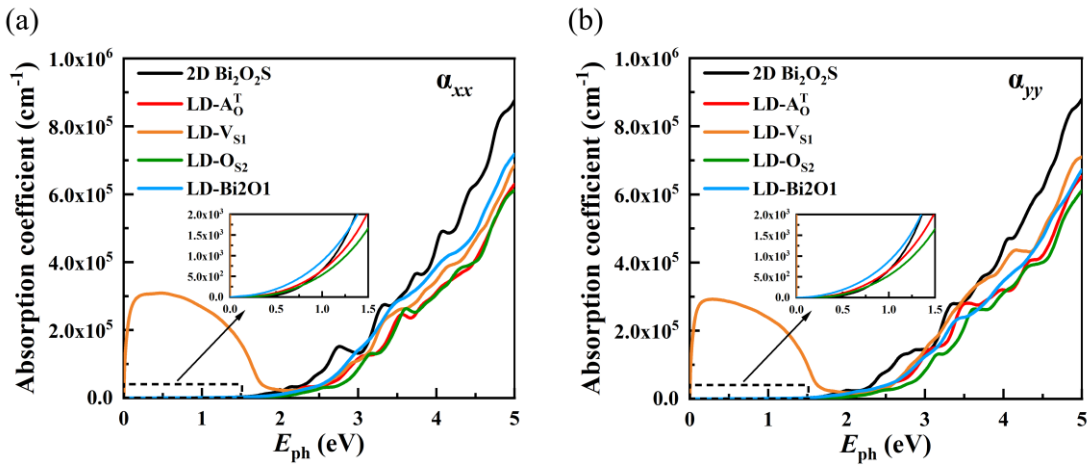

Fig. S4 The absorption coefficients of 2D Bi_2O_2S and the line defects along (a) *x*- and (b) *y*-directions.