Supporting Information

For

The structural properties for silicon-doped DBrTBT/ZnSe solar cells materials: A theoretical study

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Fig. S1. Optimized geometric structures of the DBrTBT.

Fig. S2. Optimized geometric structures of the benzene ring C(1) atom replaced by Si atom in the DBrTBT, DBrTBT-Si(1) for short.

Fig. S3. Optimized geometric structures of the benzene ring C(2) atom replaced by Si atom in the DBrTBT, DBrTBT-Si(2) for short.

Fig. S4. Optimized geometric structures of the benzene ring C(6) atom replaced by Si atom in the DBrTBT, DBrTBT-Si(6) for short.

Fig. S5. Mulliken atomic charges of the DBrTBT.

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Fig.S9. Mulliken atomic charges of part of the atoms on the ZnSe(100)-DBrTBT.

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Fig. S12. Mulliken atomic charges of part of the atoms on the ZnSe(111)-DBrTBT-Si(1).

Fig. S13. Electron density plots (EDPs) of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO).

Table S1. The origin data of absorption bands for the DBrTBT and DBrTBT-Si(x) (x=1, 2, 6) by GGA/PW91 function and RPA TD-DFT method.
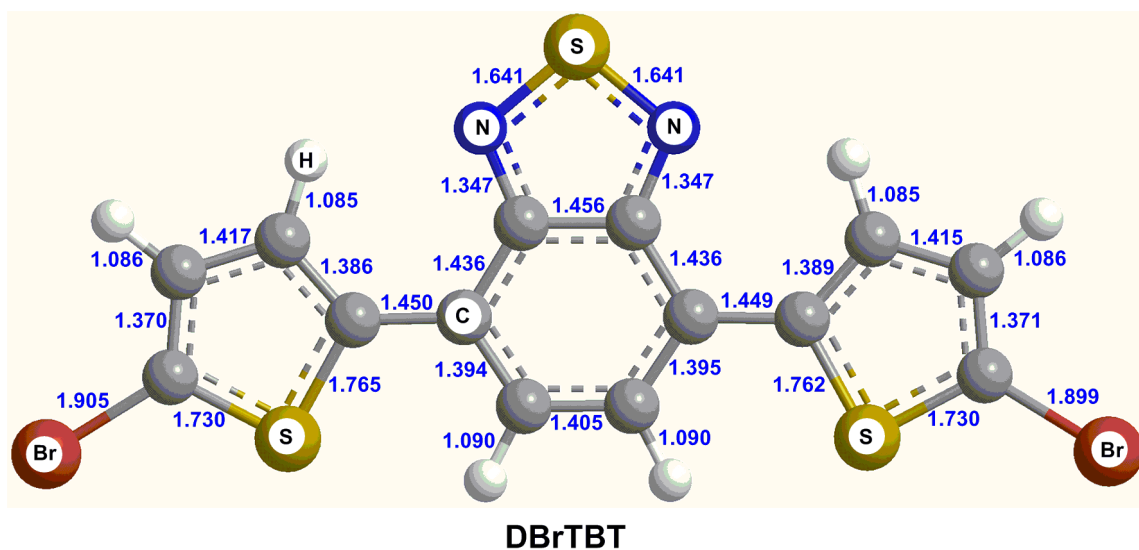
DBrTBT

Fig. S1. Optimized geometric structures of the DBrTBT. The structural parameters were clearly labeled. The unit of bond length is Å.
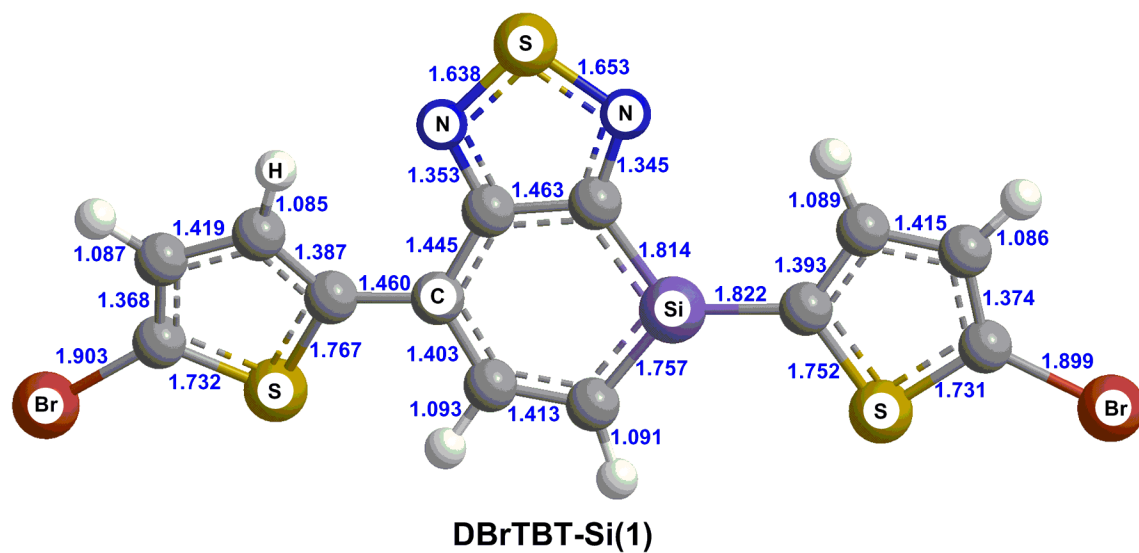

DBrTBT-Si(1)

Fig. S2. Optimized geometric structures of the benzene ring C(1) atom replaced by Si atom in the DBrTBT, DBrTBT-Si(1) for short. The structural parameters were clearly labeled. The unit of bond length is Å.
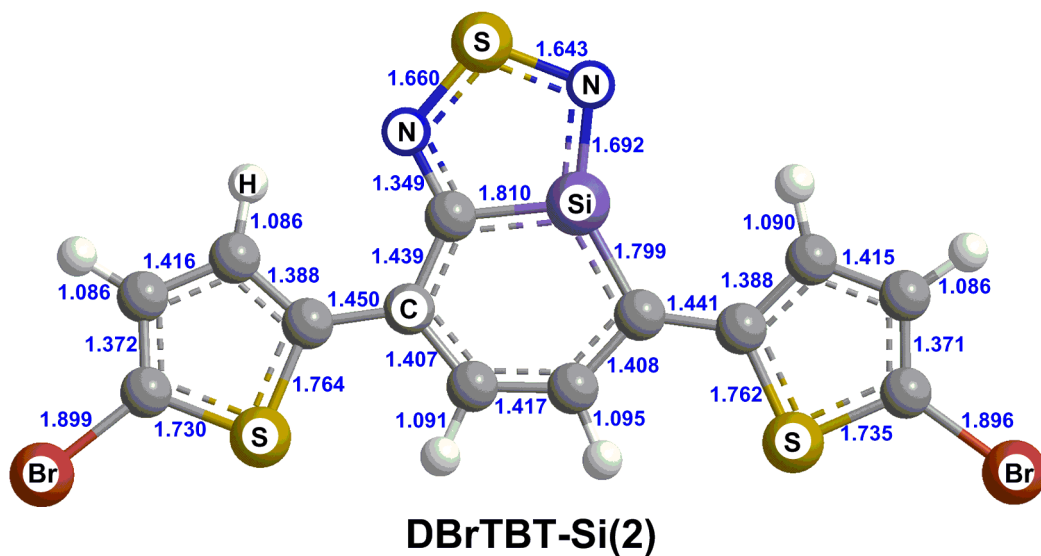
DBrTBT-Si(2)

Fig. S3. Optimized geometric structures of the benzene ring C(2) atom replaced by Si atom in the DBrTBT, DBrTBT-Si(2) for short. The structural parameters were clearly labeled. The unit of bond length is Å.
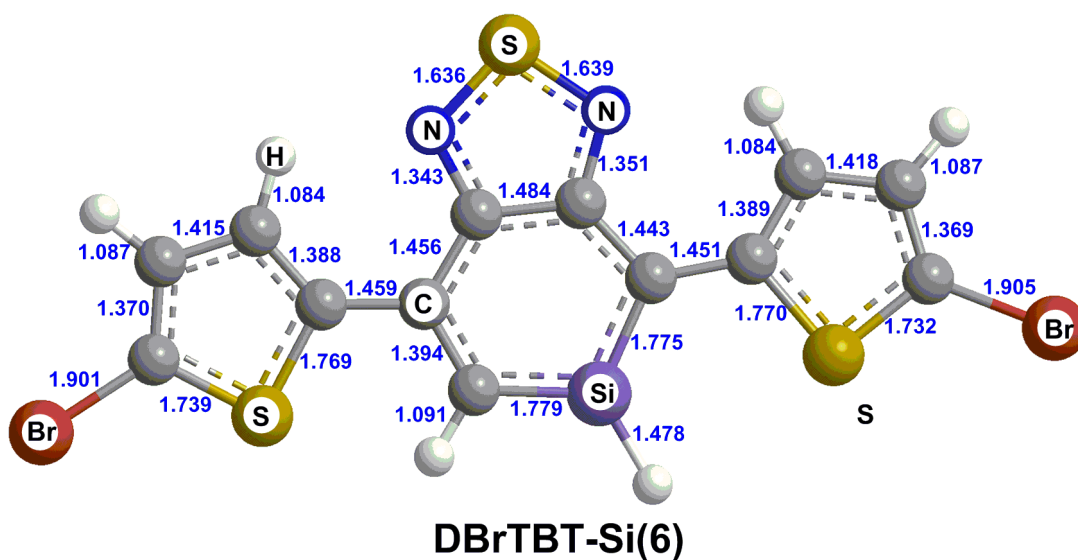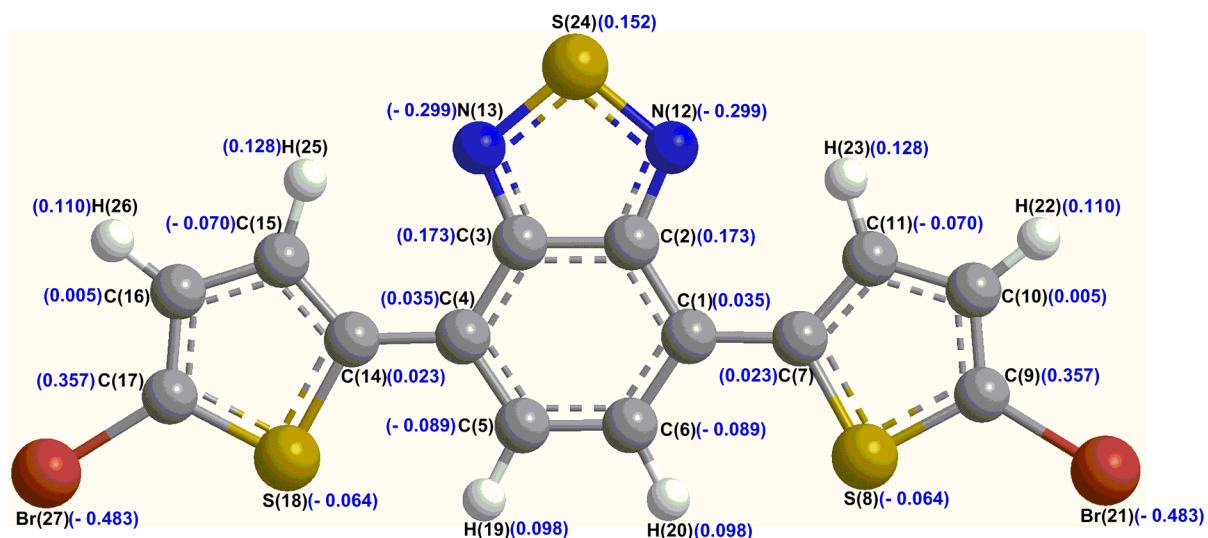

DBrTBT-Si(6)

Fig. S4. Optimized geometric structures of the benzene ring C(6) atom replaced by Si atom in the DBrTBT, DBrTBT-Si(6) for short. The structural parameters were clearly labeled. The unit of bond length is Å.
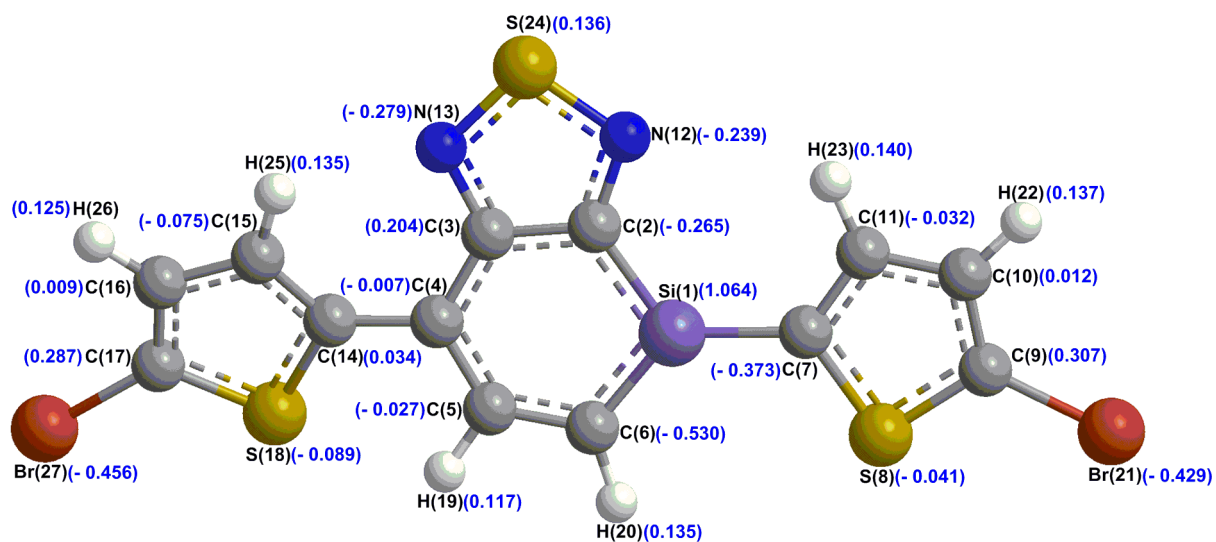
DBrTBT

Fig. S5. Mulliken atomic charges of the DBrTBT. The unit of charge is e.

DBrTBT-Si(1)

Fig. S6. Mulliken atomic charges of the DBrTBT-Si(1). The unit of charge is e.

ZnSe(100)

Fig. S7. Mulliken atomic charges of the first layer Zn and the second layer Se atoms on the ZnSe(100). The unit of charge is e.

ZnSe(111)

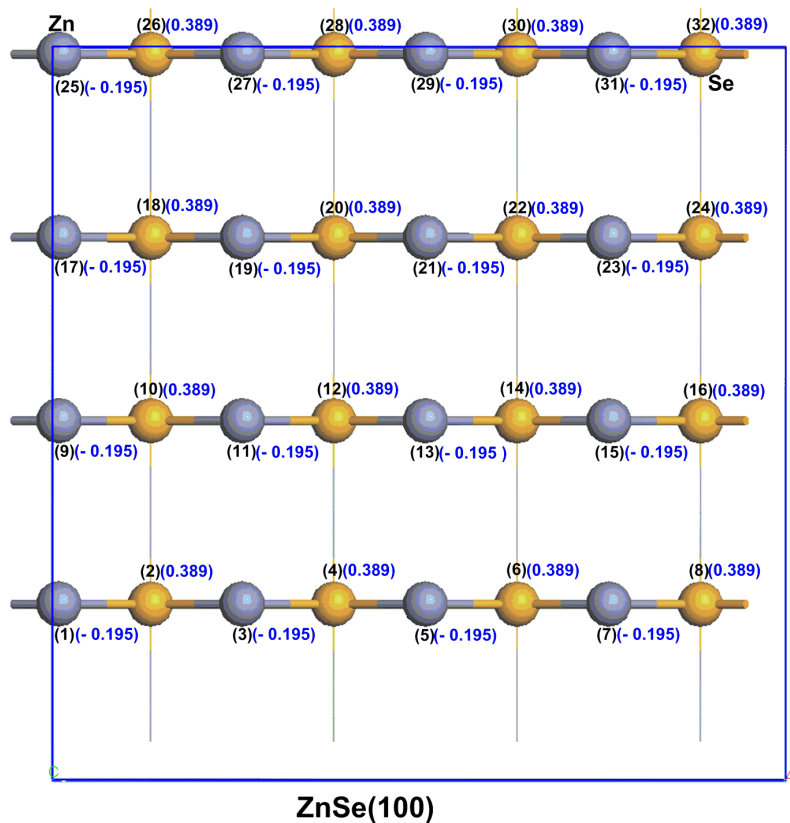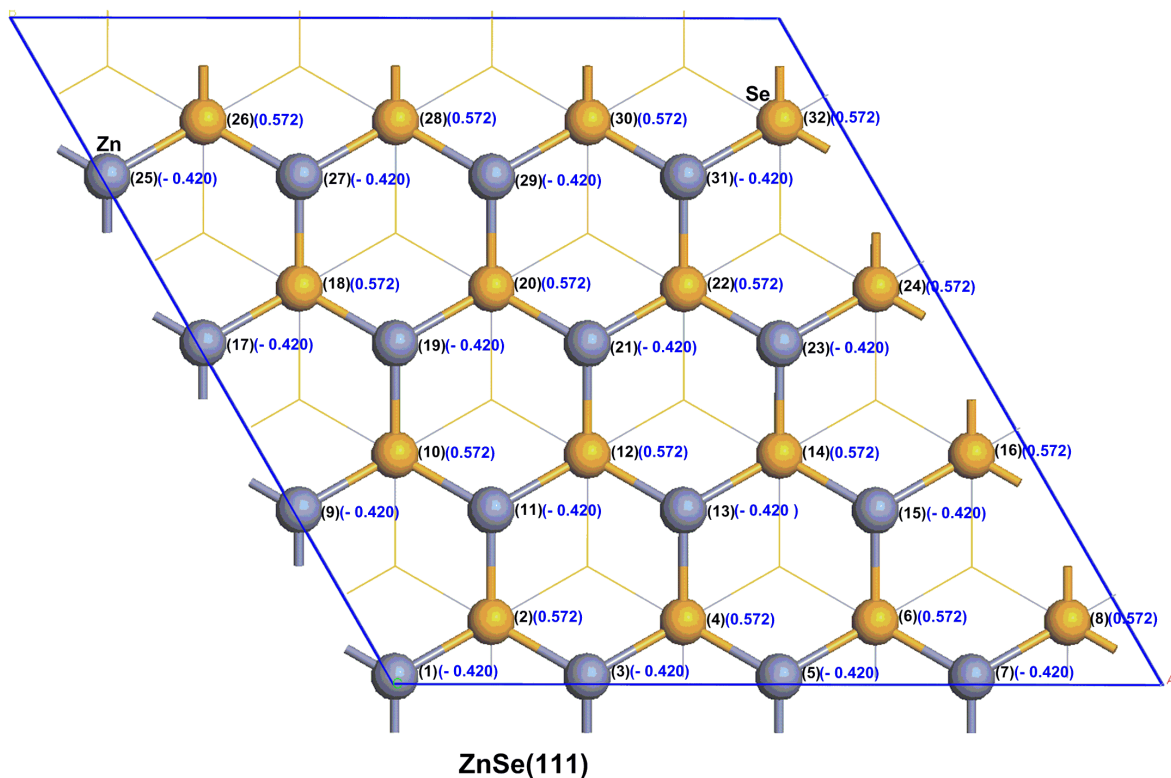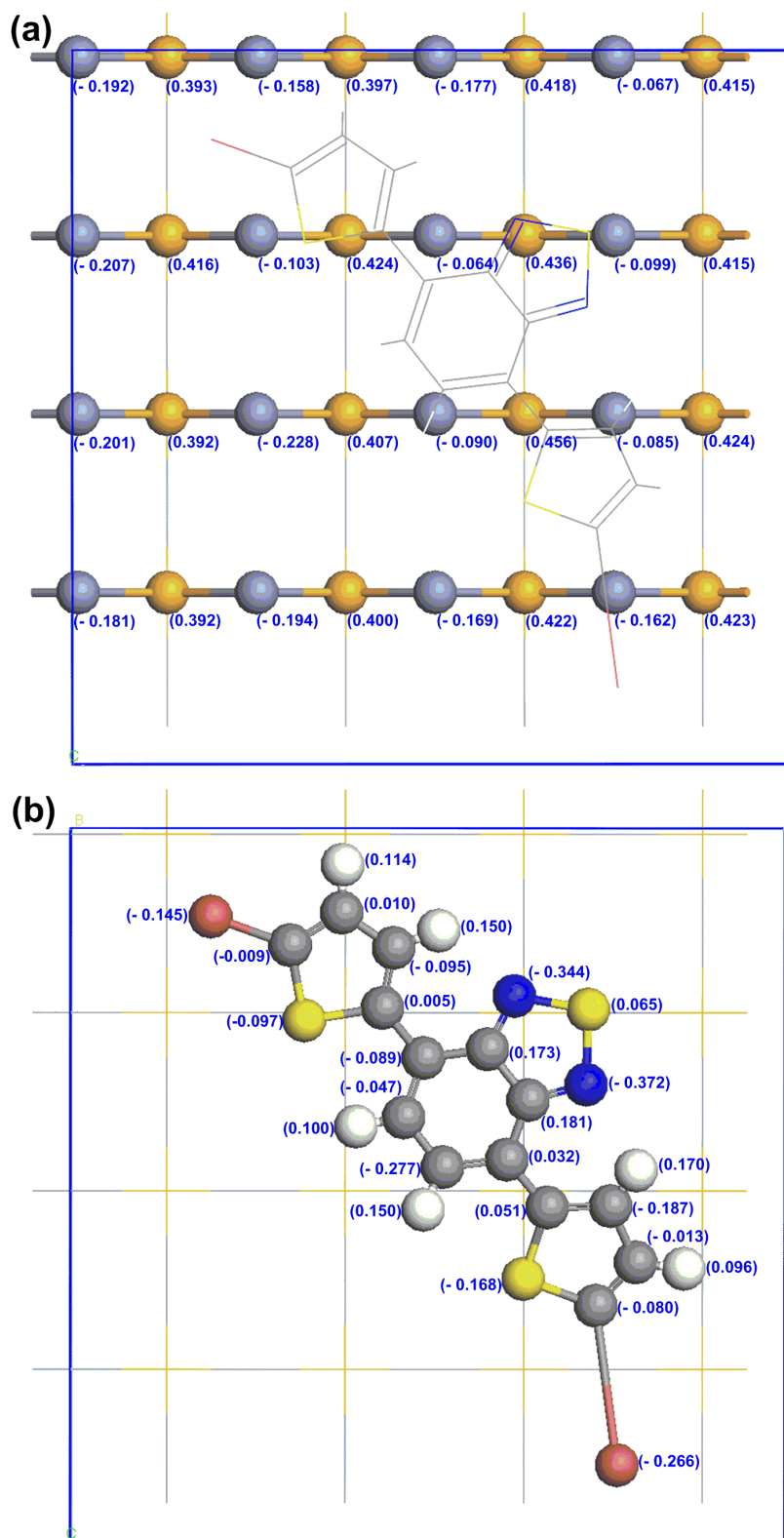**Fig. S8.** Mulliken atomic charges of the first layer Zn and the second layer Se atoms on the ZnSe(111). The unit of charge is e.

(a)

(- 0.192) (0.393) (- 0.158) (0.397) (- 0.177) (0.418) (- 0.067) (0.415)

(- 0.207) (0.416) (- 0.103) (0.424) (- 0.064) (0.436) (- 0.099) (0.415)

(- 0.201) (0.392) (- 0.228) (0.407) (- 0.090) (0.456) (- 0.085) (0.424)

(- 0.181) (0.392) (- 0.194) (0.400) (- 0.169) (0.422) (- 0.162) (0.423)

(b)

(0.114)
(0.010)
(- 0.145)
(0.150)
(-0.009)
(- 0.095)
(- 0.344)
(-0.097)
(0.005)
(0.065)
(- 0.089)
(0.173)
(- 0.047)
(- 0.372)
(0.100)
(0.181)
(- 0.277)
(0.032)
(0.170)
(0.150)
(0.051)
(- 0.187)
(- 0.013)
(0.096)
(- 0.168)
(- 0.080)
(- 0.266)

ZnSe(100)-DBrTBT

Fig. S9. Mulliken atomic charges of part of the atoms on the ZnSe(100)-DBrTBT. The unit of charge is e. (a) Mulliken atomic charges of the first layer Zn and the second layer Se atoms on the ZnSe(100) surface and (b) Mulliken atomic charges of the DBrTBT.

(a)

(0.405) (- 0.797) (0.471) (- 0.802) (0.396) (- 0.799) (0.392) (- 0.798)

(0.380) (- 0.799) (0.572) (- 0.781) (0.656) (- 0.823) (0.495) (- 0.791)

(0.391) (- 0.796) (0.406) (- 0.821) (0.351) (- 0.814) (0.446) (- 0.797)

(0.394) (- 0.795) (0.380) (- 0.796) (0.521) (- 0.793) (0.442) (- 0.796)

(b)

(0.123)

(- 0.492) (0.013)

(0.273) (0.141)

(- 0.099)

(- 0.450)

(- 0.098) (0.024) (0.081)

(0.202)

(- 0.018) (- 0.281)

(0.107) (- 0.221)

(- 0.038) (1.081)

(- 0.502) (0.129)

(0.117) (- 0.353) (- 0.046)

(0.004)

(- 0.092) (0.127)

(0.300)

(- 0.473)
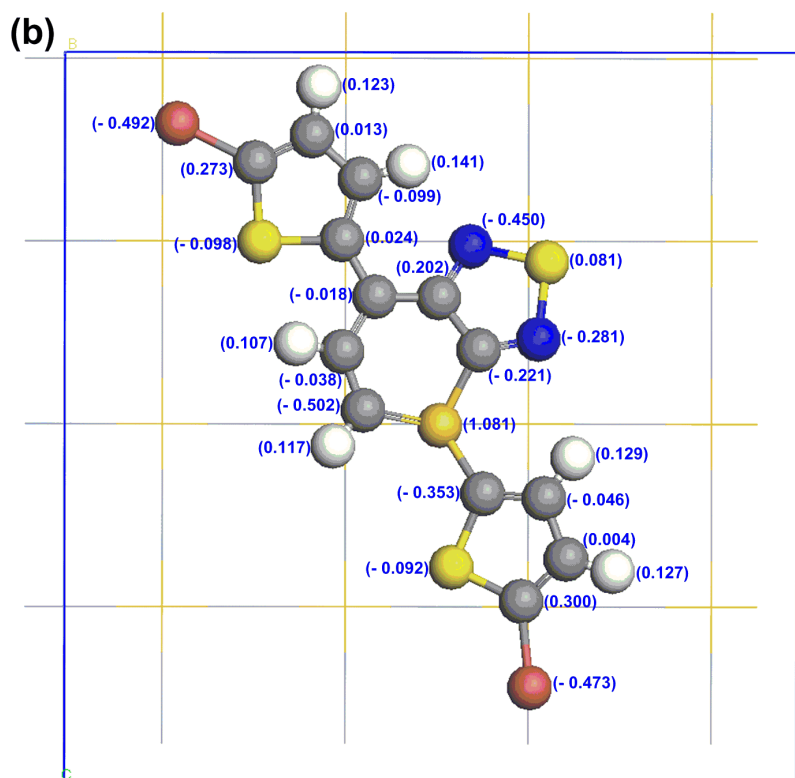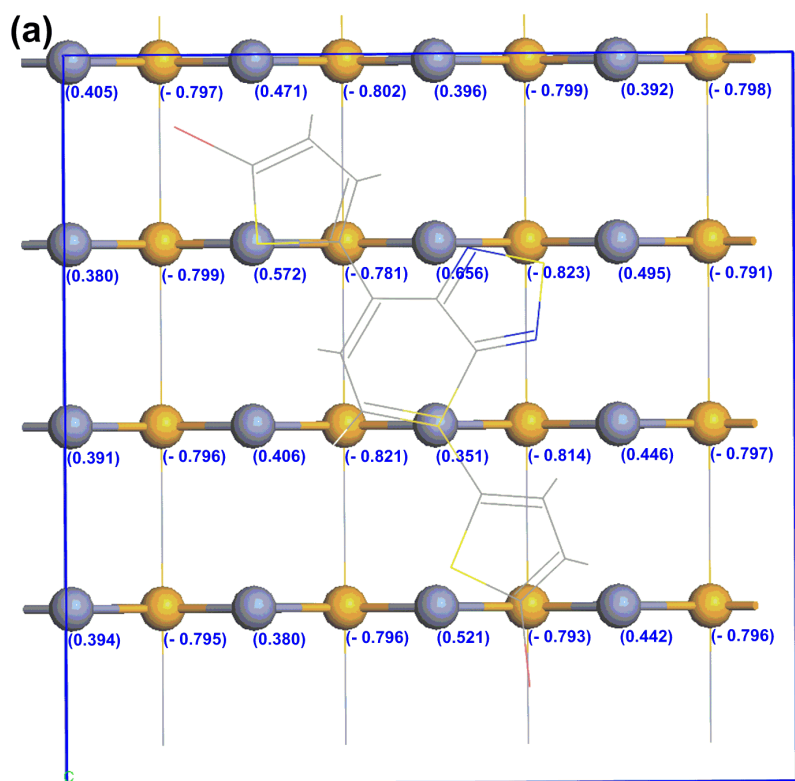
ZnSe(100)-DBrTBT-Si(1)

Fig. S10. Mulliken atomic charges of part of the atoms on the ZnSe(100)-DBrTBT-Si(1). The unit of charge is e.　(a) Mulliken atomic charges of the first layer Zn and the second layer Se atoms on the ZnSe(100) surface and (b) Mulliken atomic charges of the DBrTBT-Si(1).
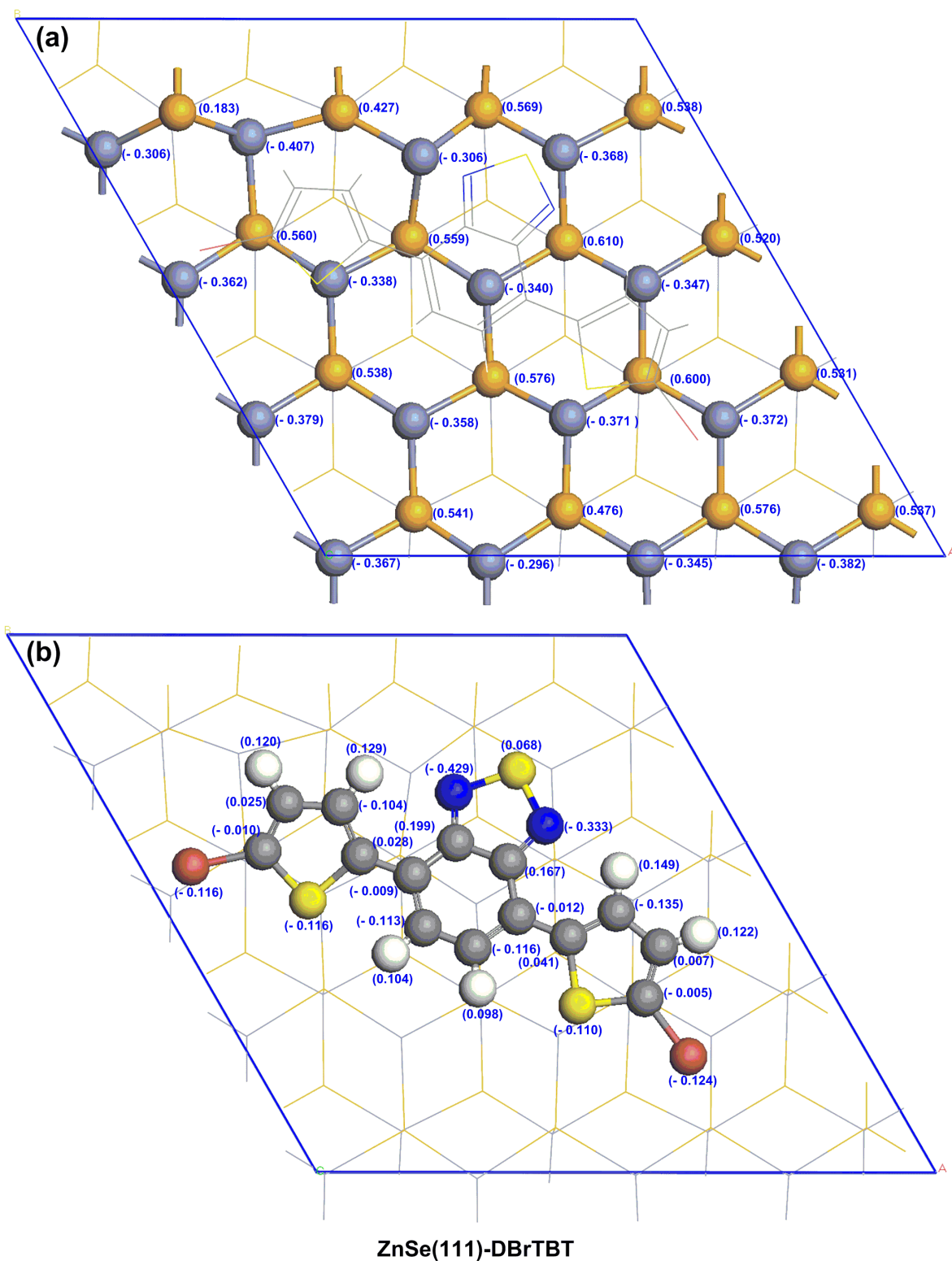
ZnSe(111)-DBrTBT

Fig. S11. Mulliken atomic charges of part of the atoms on the ZnSe(111)-DBrTBT. The unit of charge is e. (a) Mulliken atomic charges of the first layer Zn and the second layer Se atoms on the ZnSe(111) surface and (b) Mulliken atomic charges of the DBrTBT.

ZnSe(111)-DBrTBT-Si(1)

Fig. S12. Mulliken atomic charges of part of the atoms on the ZnSe(111)-DBrTBT-Si(1). The unit of charge is e. (a) Mulliken atomic charges of the first layer Zn and the second layer Se atoms on the ZnSe(111) surface and (b) Mulliken atomic charges of the DBrTBT-Si(1).
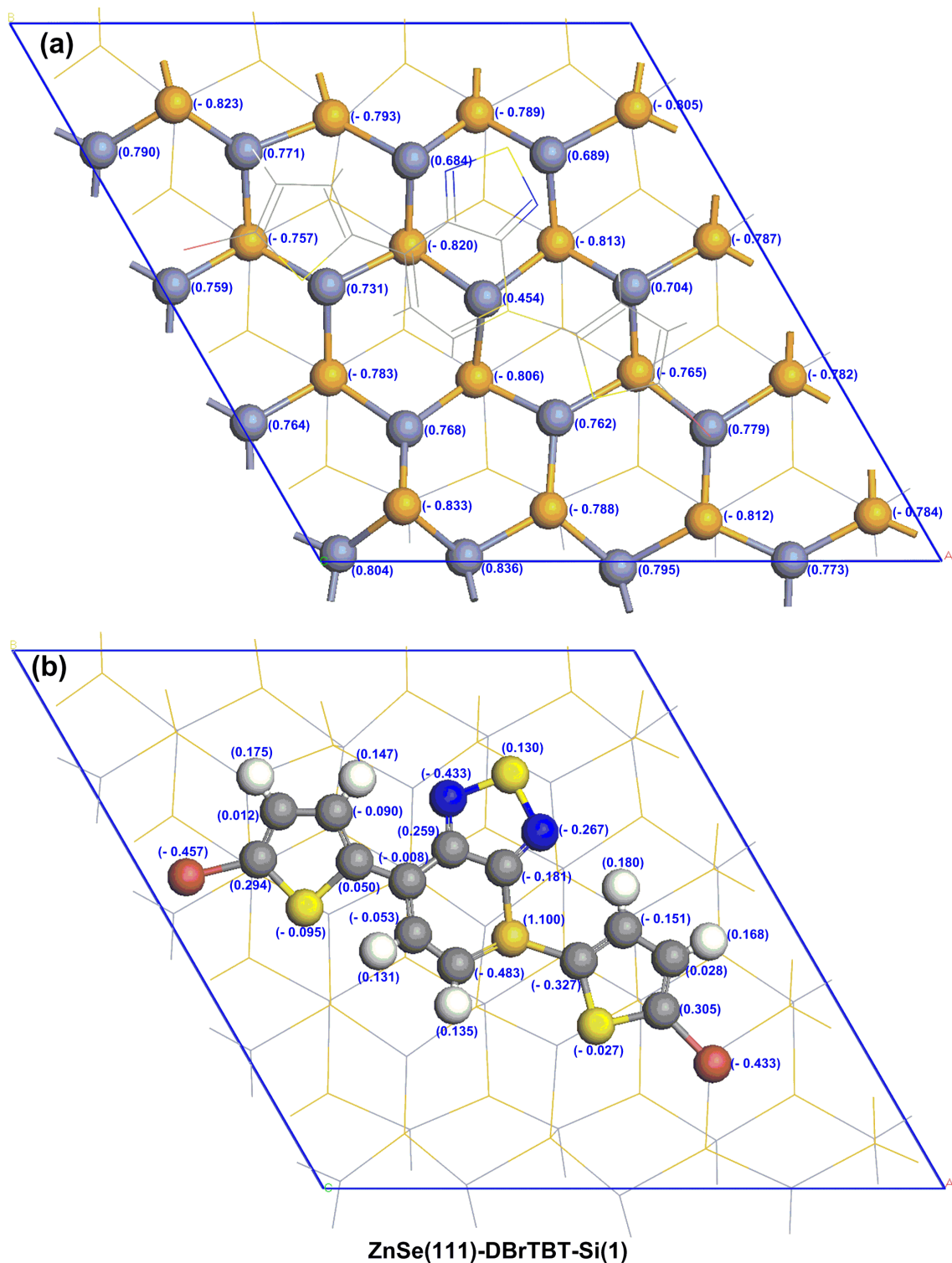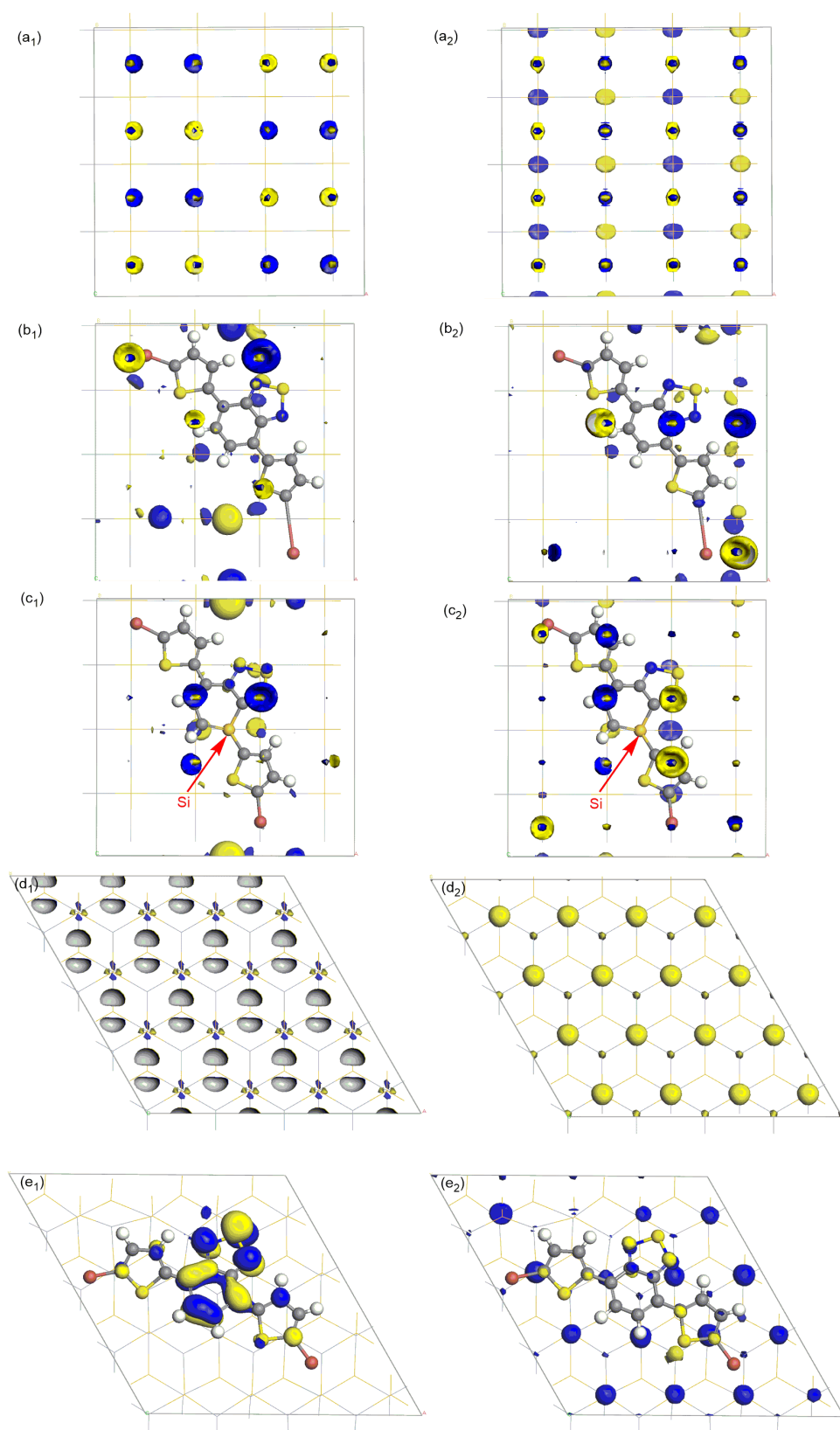
Fig. S13. Electron density plots (EDPs) of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). (a_1) ZnSe(100)-HOMO, (a_2)ZnSe(100)-LUMO, (b_1) ZnSe(100)-DBrTBT-HOMO, (b_2) ZnSe(100)-DBrTBT-LUMO, (c_1) ZnSe(100)-DBrTBT-Si(1)-HOMO, (c_2) ZnSe(100)-DBrTBT-Si(1)-LUMO, (d_1) ZnSe (111)-HOMO, (d_2) ZnSe(111)-LUMO, (e_1) ZnSe(111)-DBrTBT-HOMO, and (e_2) ZnSe(111)-DBrTBT-LUMO.

Table S1. The origin data of absorption bands for the DBrTBT and DBrTBT-Si(x) (x=1, 2, 6) by GGA/PW91 function and RPA TD-DFT method.

DBrTBT		DBrTBT-Si(1)		DBrTBT-Si(2)		DBrTBT-Si(6)	
Wavelength /nm	Strength/ a.u.	Wavelength /nm	Strength/ a.u.	Wavelength /nm	Strength/ a.u.	Wavelength /nm	Strength/ a.u.
279	0.0182	297	0.0128	315	0.0006	318	0.0001
309	0.0001	300	0.0372	320	0.0017	319	0.0018
317	0.0071	324	0.0096	328	0.0005	320	0.0366
323	0.0457	339	0.0145	331	0.0011	344	0.0022
324	0.0024	347	0.0729	339	0.0722	347	0.0009
325	0.0015	349	0.0045	353	0.0000	351	0.0293
337	0.0271	356	0.0546	367	0.0316	359	0.0076
362	0.0344	359	0.0257	371	0.0043	367	0.0016
363	0.0003	364	0.0006	384	0.5641	379	0.1790
374	0.6428	397	0.3290	409	0.0245	403	0.3517
420	0.0055	431	0.1921	444	0.0752	440	0.0184
559	0.3038	594	0.1959	574	0.3308	593	0.2744