

## 补充材料

### 氢空位簇调控啫烷的电子结构与分子掺杂\*

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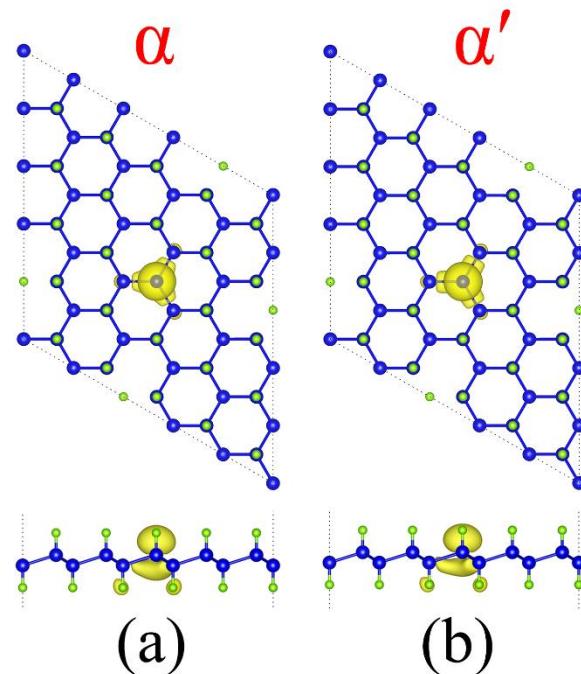


图 S1  $G_{D-IH}$  体系  $\alpha$  和  $\alpha'$  平带的能带分解电荷密度, 其中等值面设为  $0.002 e/\text{\AA}^3$

Fig. S1. Band decomposed charge density for the  $\alpha$  and  $\alpha'$  in  $G_{D-IH}/TTF$  system. The isosurface is set to  $0.002 e/\text{\AA}^3$ .

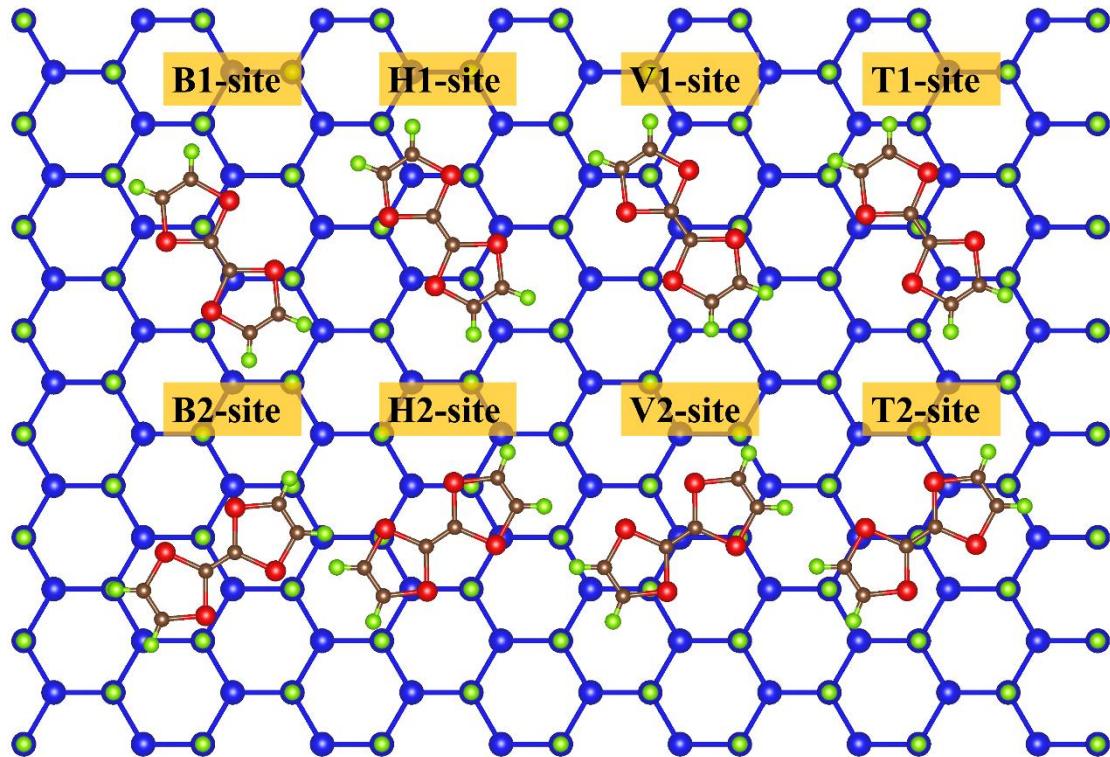


图 S2 TTF 分子在锗烷表面的八种典型吸附位，分别命名为：B1-site, B2-site, H1-site, H2-site,

V1-site, V2-site, T1-site, T2-site

Fig. S2. Eight typical adsorption sites of TTF molecule on germanane surface, named as B1-site,

B2-site, H1-site, H2-site, V1-site, V2-site, T1-site and T2-site, respectively.

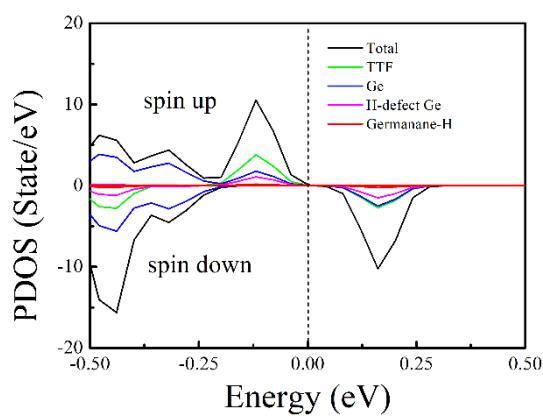


图 S3  $G_{D-1H}$ /TTF 的投影态密度图

Fig. S3. Projected density of states of  $G_{D-1H}$ /TTF.