补充材料

氢空位簇调控锗烷的电子结构与分子掺杂*

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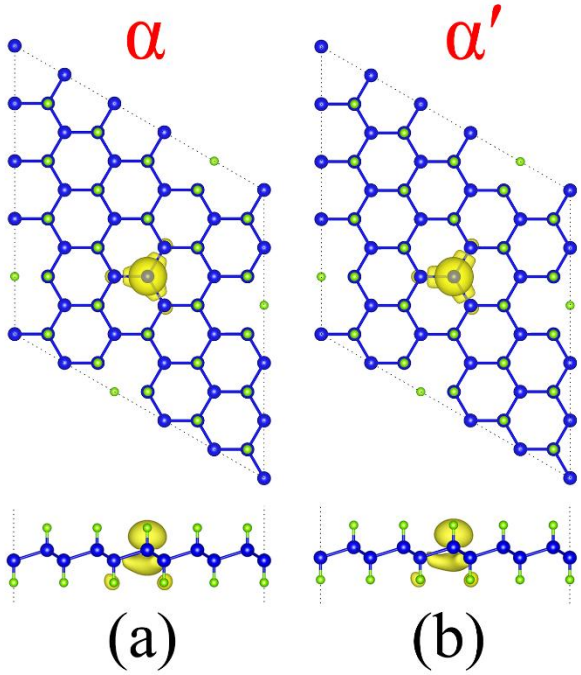

图 S1 $G_{D\text{-}1H}$ 体系α和α'平带的能带分解电荷密度，其中等值面设为 0.002 e/Å^3

Fig. S1. Band decomposed charge density for the α and α' in $G_{D\text{-}1H}$/TTF system. The isosurface is set to 0.002 e/Å^3.

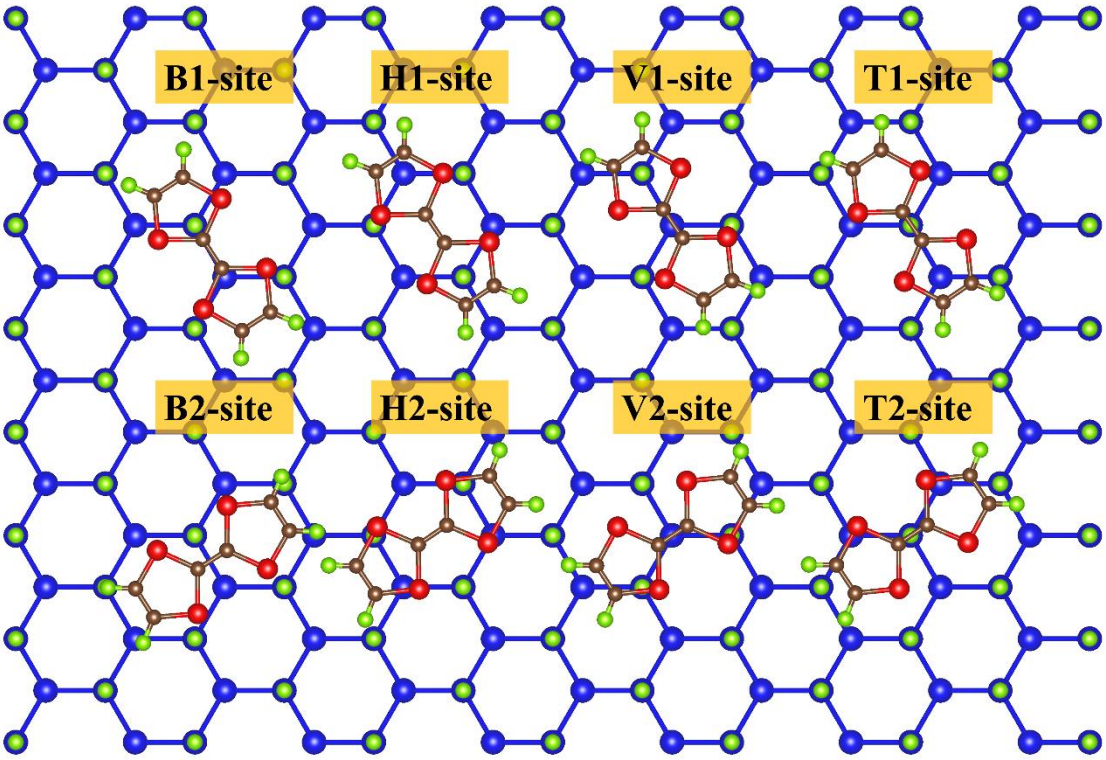

图 S2 TTF 分子在锗烷表面的八种典型吸附位，分别命名为：B1-site, B2-site, H1-site, H2-site, V1-site, V2-site, T1-site, T2-site

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.

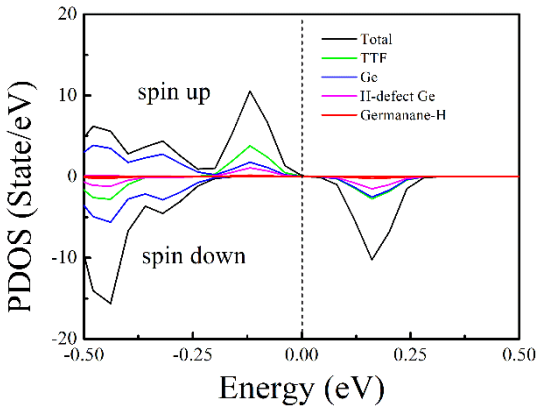

图 S3 $G_{D\text{-}1H}$/TTF 的投影态密度图

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