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SUPPLEMENTAL MATERIALS

Tuning the magnetic and electronic properties of strontium titanate by carbon doping

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Table T1 Average contribution of MM (μB) for Sr, Ti, and O atoms in FM and AFM states in different $SrTiO_{2.75}C_{0.25}$ configurations.

Configuration	MM_{Sr} (FM/AFM)	MM_{Ti} (FM/AFM)	MM_O (FM/AFM)
A	0/0	0/0	0/0
B	0.010/0.006	0.002/0.004	0.031/0.007
C	0.017/0	0.005/0	0.038/0
D	0.018/0	0.008/0	0.035/0
E	0.015/0	0.014/0	0.036/0
F	0.019/0	0.005/0	0.038/0
G	0.017/0	0.007/0	0.038/0

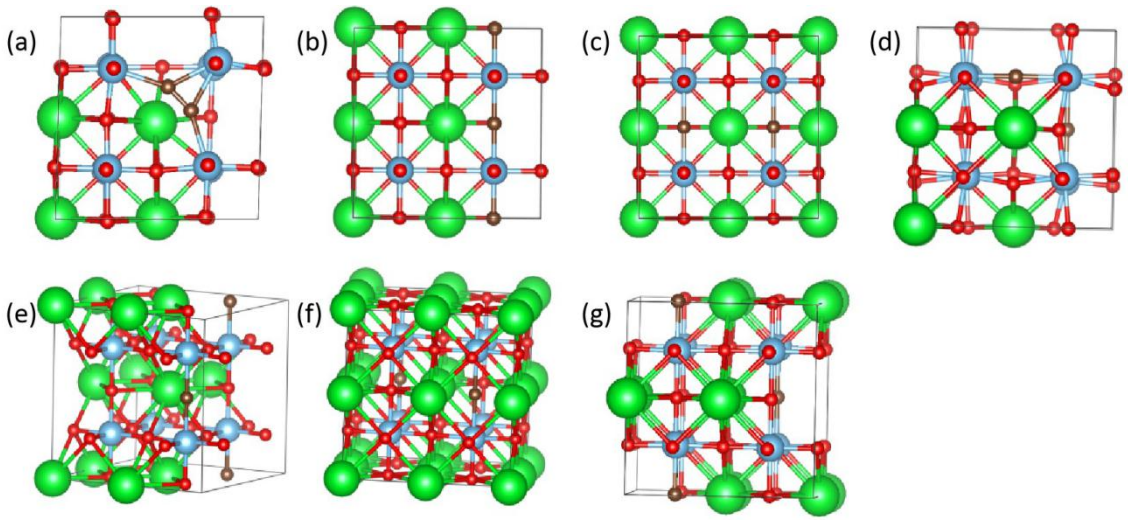

Fig. S1 (a-g) The relaxed structures in configurations A-G, with C-C distance ranging from 1.297 Å to 6.868 Å. Color codes: green for Sr, red for O atoms, violet red for Ti, saddle brown for dopant carbon atoms.

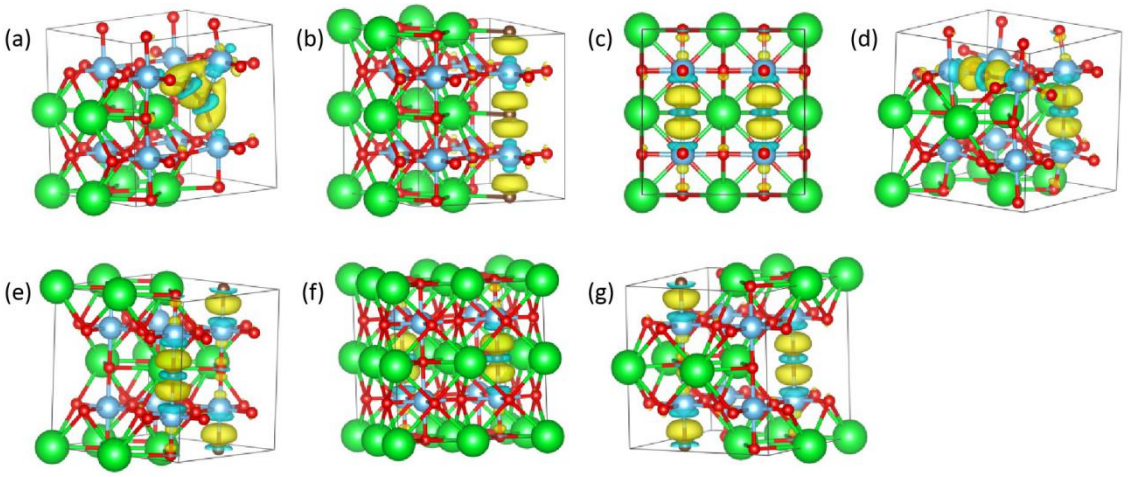

Fig. S2 (a-g) The charge different density in configurations A-G. The isosurface level value is set as 0.005 e/Å^3, and the yellow and blue violet areas represent charge accumulation and charge depletion, respectively. Color codes: green for Sr, red for O atoms, violet red for Ti, saddle brown for dopant carbon atoms.

Table T2 Average contribution of MM (μB) for Sr, Ti, and O atoms in FM and AFM states in different $SrTiO_{2.75}C_{0.25}$ configurations calculated by the GGA+*U* (*U* = 5.8 eV) method.

Configuration	MM_{Sr} (FM/AFM)	MM_{Ti} (FM/AFM)	MM_O (FM/AFM)
A	0/0	0/0	0/0
B	0.012/0	0.036/0	0.030/0
C	0.017/0	0/0	0.030/0
D	0.016/0	0/0	0.032/0
E	0.017/0	0/0	0.029/0
F	0.019/0	-0.004/0	0.031/0
G	0.017/0	-0.003/0	0.032/0