

Supplementary Information for

Ti₄-Decorated B/N-Doped Graphene as High-

Capacity Hydrogen Storage Material: A DFT Study

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Fig. S1. The isosurfaces of the EDD for Ti decorated graphene (a) Ti/Gr, (b) Ti/BGr, and (c) Ti/NGr are presented. In the EDD plots, the red and yellow colors represent electron accumulation and depletion regions, respectively. The isosurfaces of EDD is taken to be $0.02 \text{ e}/\text{\AA}^3$.

Fig. S2. All possible optimized configurations of the Ti_4 cluster decorated on pristine graphene.

Fig. S3. All possible optimized configurations of the Ti_4 cluster decorated on B-doped graphene.

Fig. S4. All possible optimized configurations of the Ti_4 cluster decorated on N-doped graphene.

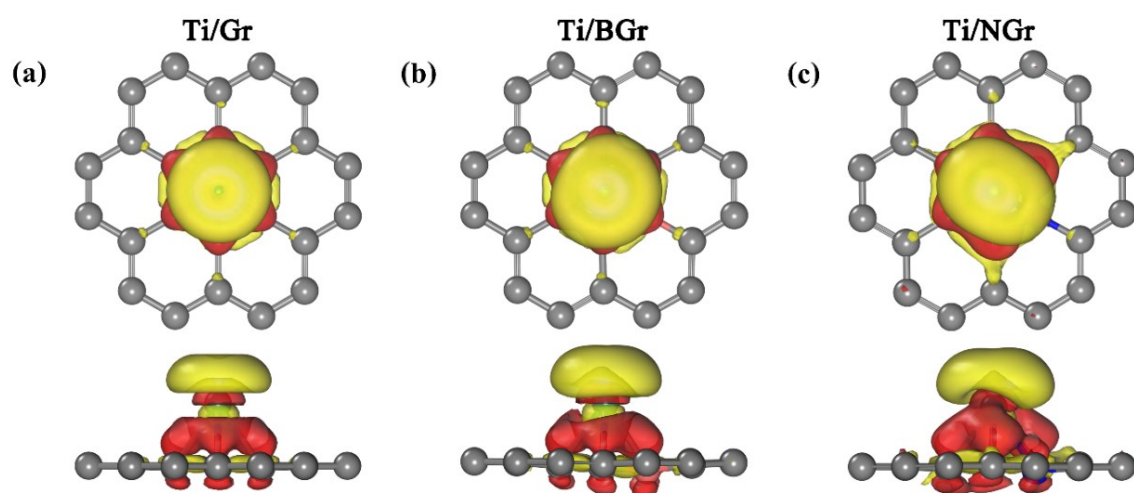


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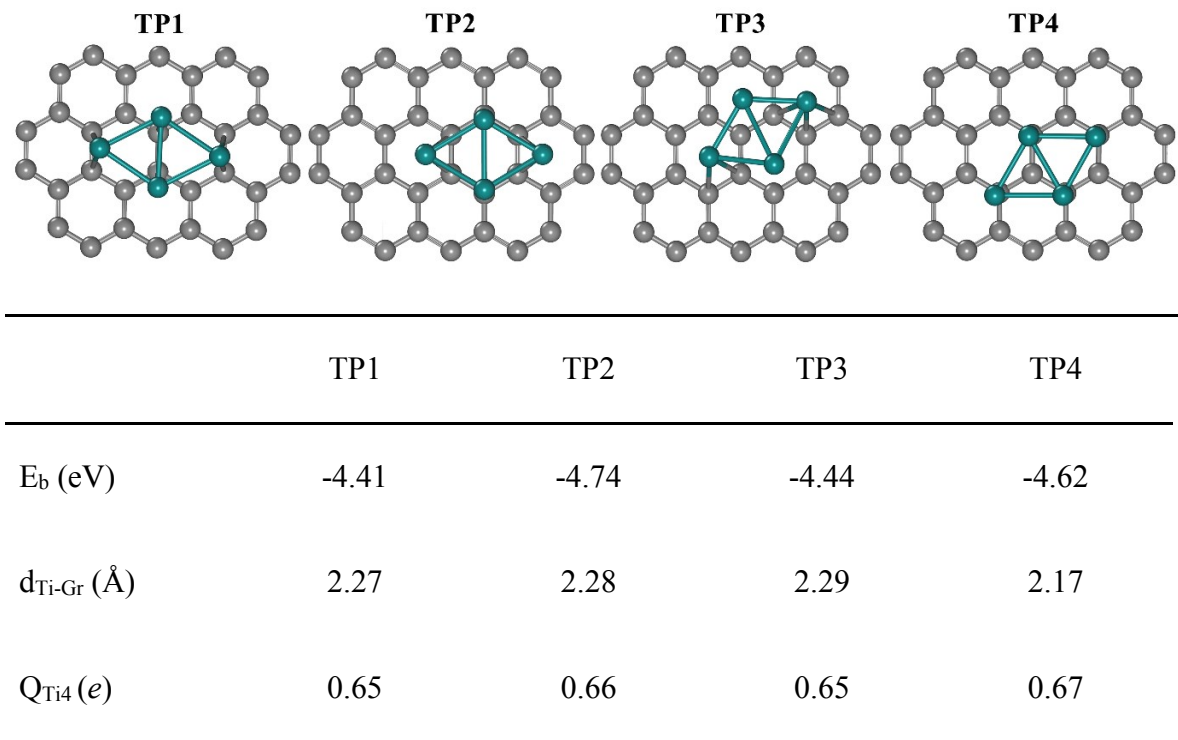


Fig. S2. All possible optimized configurations of the Ti_4 cluster decorated on pristine graphene.

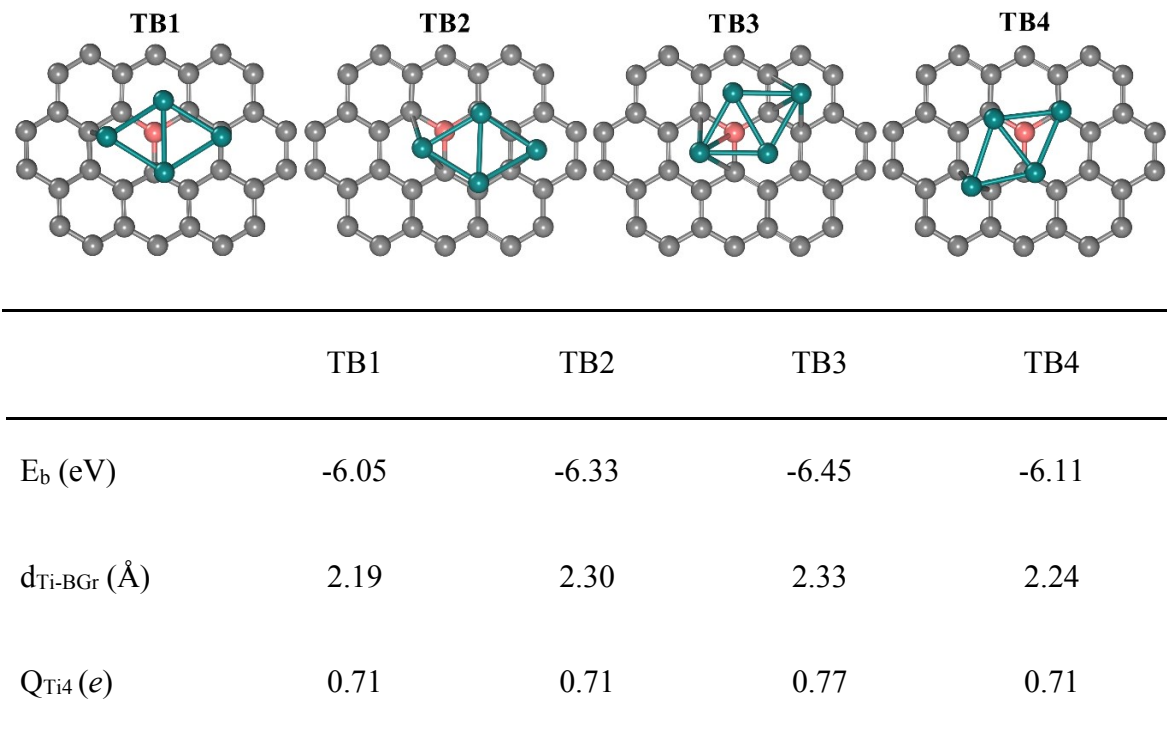
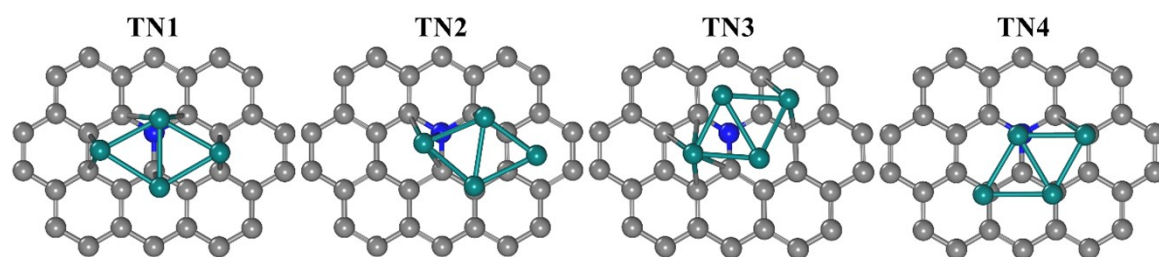


Fig. S3. All possible optimized configurations of the Ti_4 cluster decorated on B-doped graphene.



	TN1	TN2	TN3	TN4
E_b (eV)	-4.33	-4.52	-4.33	-4.79
$d_{\text{Ti-NGr}}$ (Å)	2.25	2.24	2.29	2.18
Q_{Ti4} (e)	0.65	0.65	0.64	0.67

Fig. S4. All possible optimized configurations of the Ti_4 cluster decorated on N-doped graphene.