Supporting Information

First-principles study on the structures and electronic properties of graphene-supported Ni_n (n= 1 - 6) clusters

Wei Song[1], Jin-long Wang[1], Bin Wang[1], Wei-ping Hu[3,*], Ying Wang[2,*]

[1]*Physics and Electronic Engineering Department, Xinxiang University, Xinxiang, 453003, P.R.China*

[2]*State Key Laboratory of Rare Earth Resource Utilization, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun, 130022, P.R.China*

[3]*College of Chemistry and Chemical Engineering, Henan University, Kaifeng, 475004, P.R.China*

***Corresponding authors:**
E-mail: 48848990@qq.com(Wei-ping Hu)
***Corresponding authors:**
E-mail: ywang_2012@ciac.jl.cn (Ying Wang)

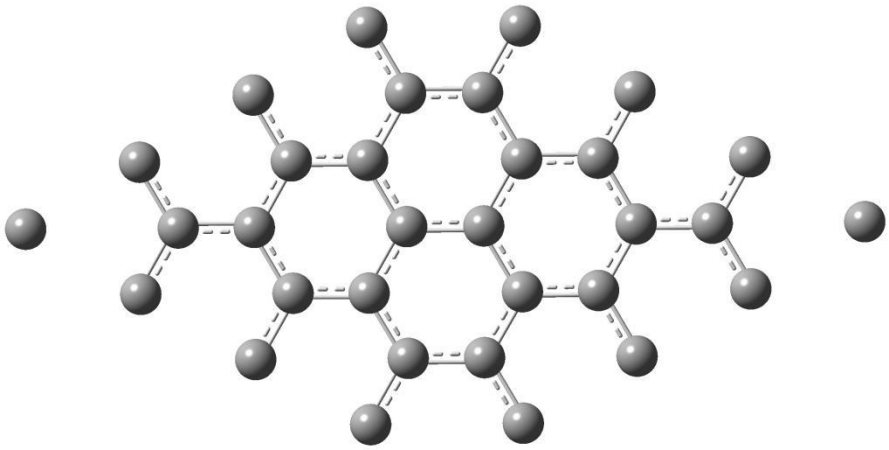

Fig. S1. The optimized structure of the 4×4 pristine graphene at the DFT-PBE level.

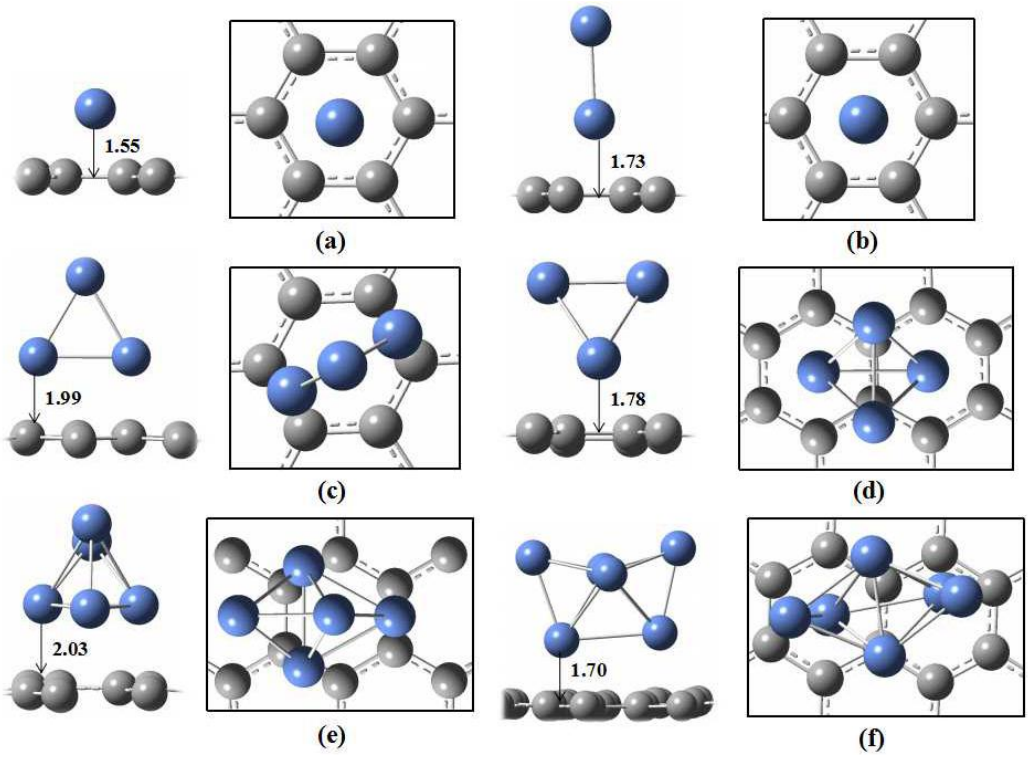

Fig. S2. The most stable structures and average distance of adsorbed (a) Ni_1 (b) Ni_2 (c) Ni_3 (d) Ni_4 (e)Ni_5 (f) Ni_6 clusters on 5% strained graphene (SG5). The blue color represents Ni atom and gray color represents C atom.

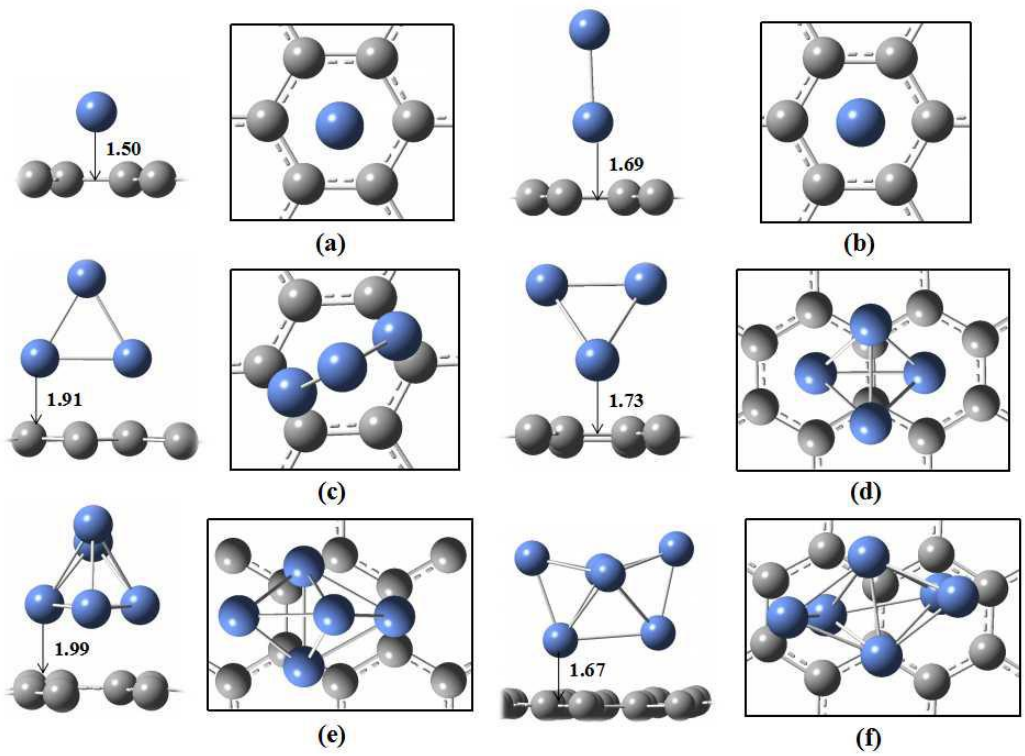

Fig. S3. The most stable structures and average distance of adsorbed (a) Ni_1 (b) Ni_2 (c) Ni_3 (d) Ni_4 (e)Ni_5 (f) Ni_6 clusters on 10% strained graphene (SG10). The blue color represents Ni atom and gray color represents C atom.

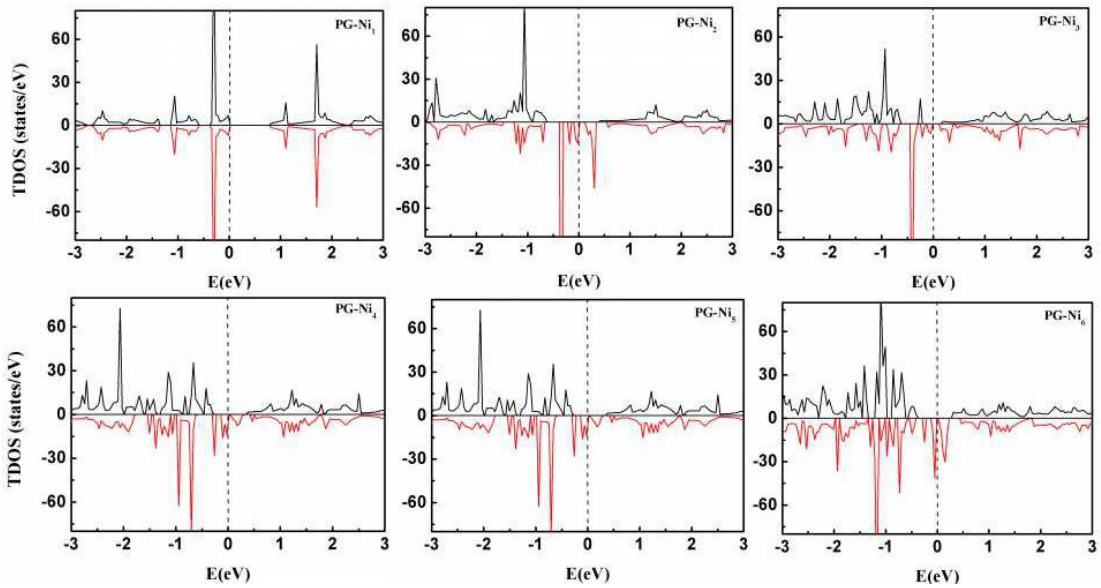

Fig. S4. The total density of states (TDOS) for pristine (PG) graphene.

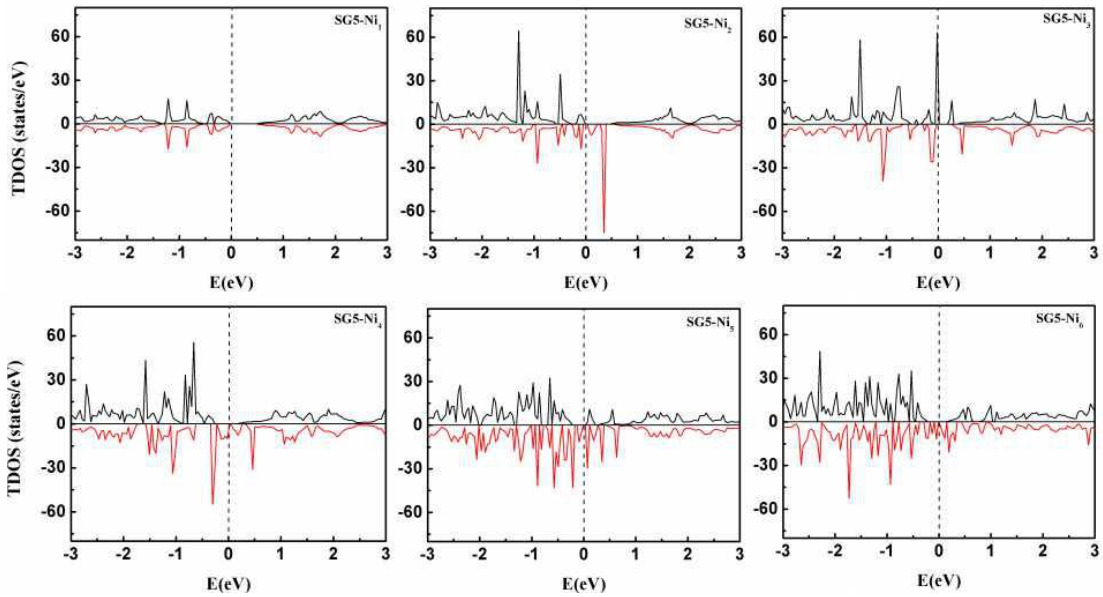

Fig. S5. The total density of states (TDOS) for 5% strained (SG5) graphene.

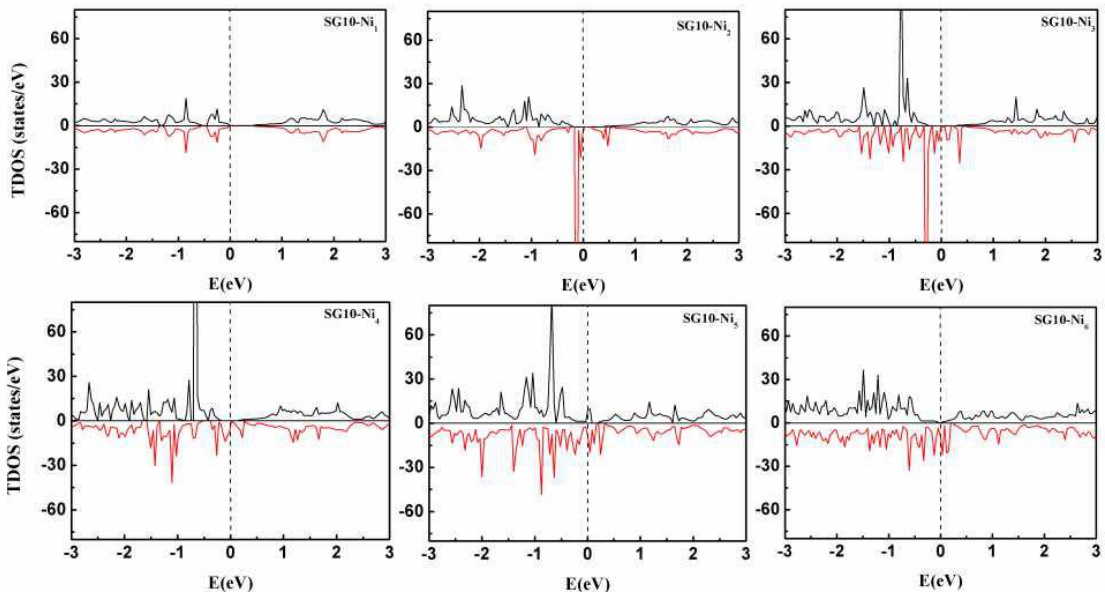

Fig. S6. The total density of states (TDOS) for 10% strained (SG10)graphene.

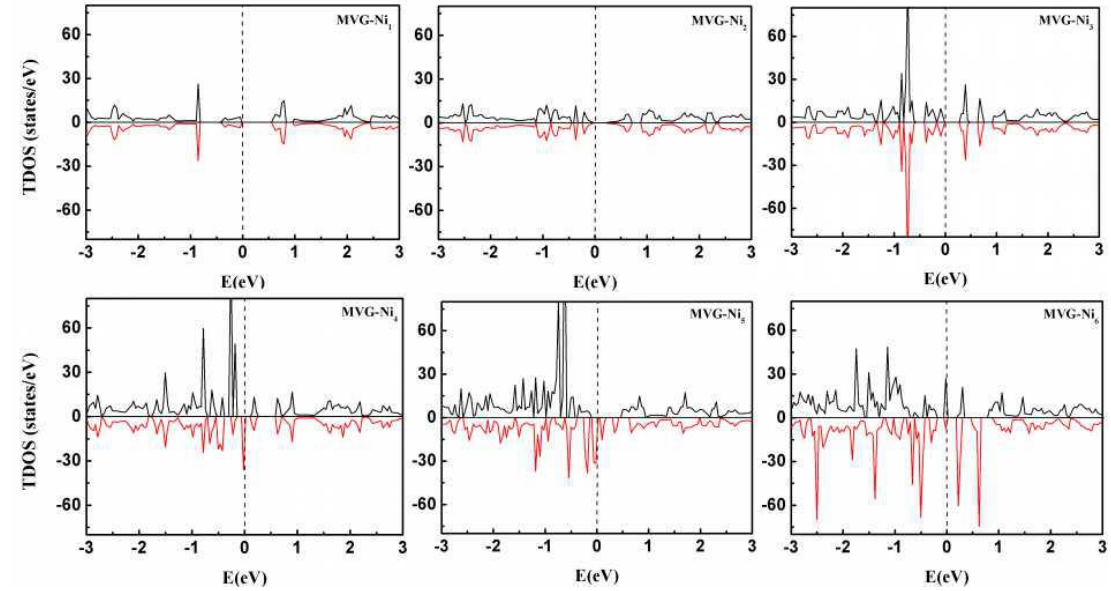

Fig. S7. The total density of states (TDOS) for monovacancy (MVG) defective graphene.

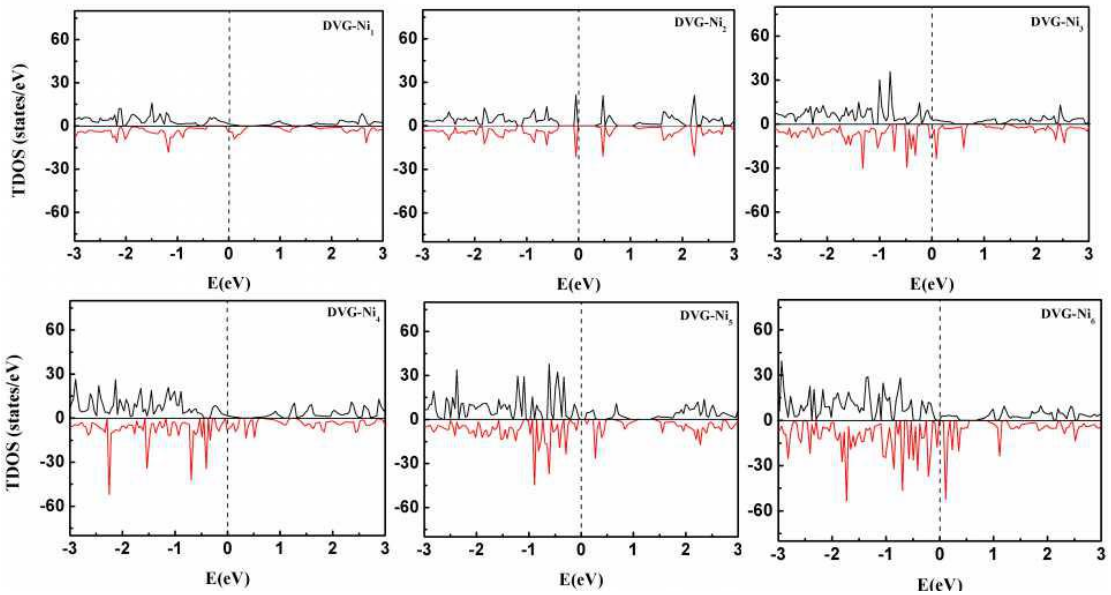

Fig. S8. The total density of states (TDOS) for divacancy (DVG) defective graphene.