Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A

Supporting Information

Introduction of Nitrogen with Controllable Configuration into Graphene *via* Vacancies and Edges

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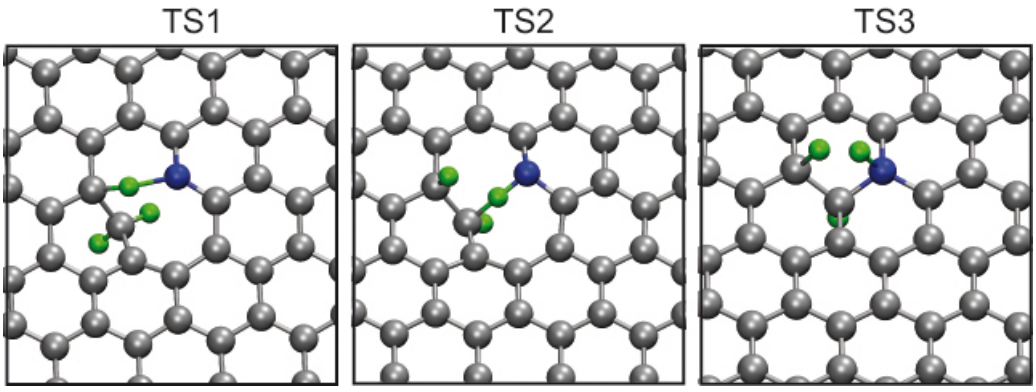

Figure S1. Transition states in the change of the configuration of nitrogen from NH-CH_2 to a graphitic-N at a single vacancy. The reaction path is shown in Figure 4 in the main text.

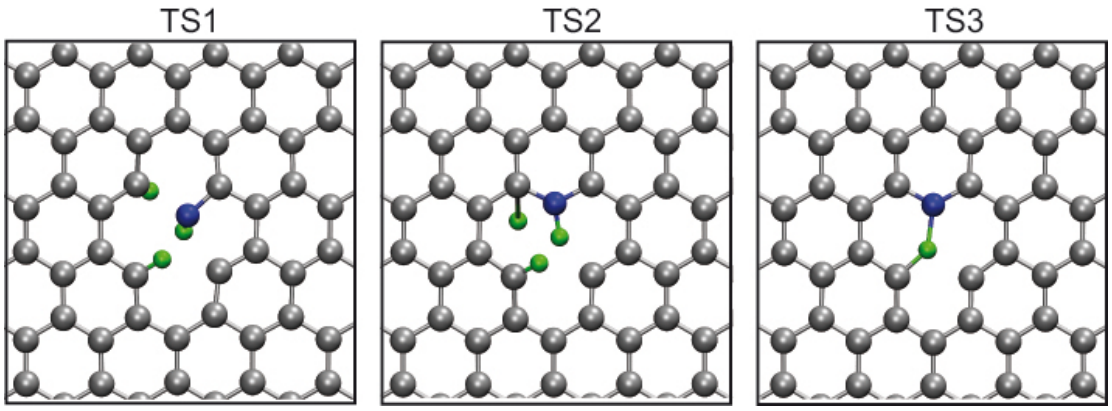

Figure S2. Transition states in the change of the nitrogen configuration from pyrrolic-N to pyridinic-N at a divacancy by desorption of a H_2 molecule. The reaction path is shown in Figure 6 in the main text.

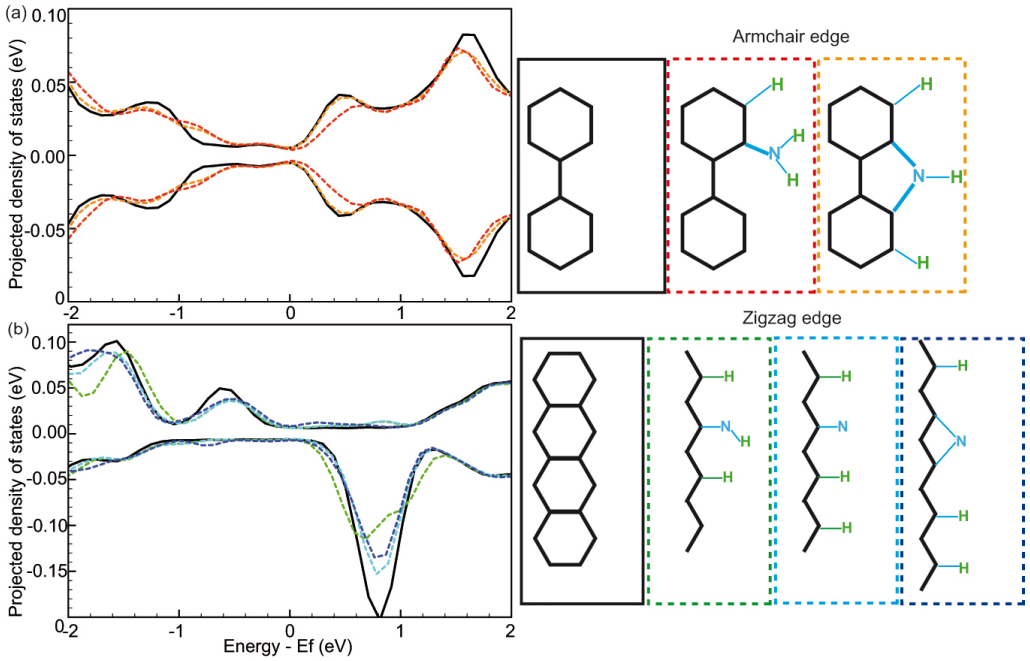

Figure S3. Projected density of states onto carbon atoms in N-doped graphene armchair ribbon (a) and zigzag ribbon (b). The different configurations are schematically shown on the right panel. At the armchair and zigzag edges, the covalent binding of nitrogen and hydrogen cause minor doping effect.