Supporting Information for

Graphene adlayer growth between nonepitaxial graphene and Ni(111) substrate: a promising theoretical scheme

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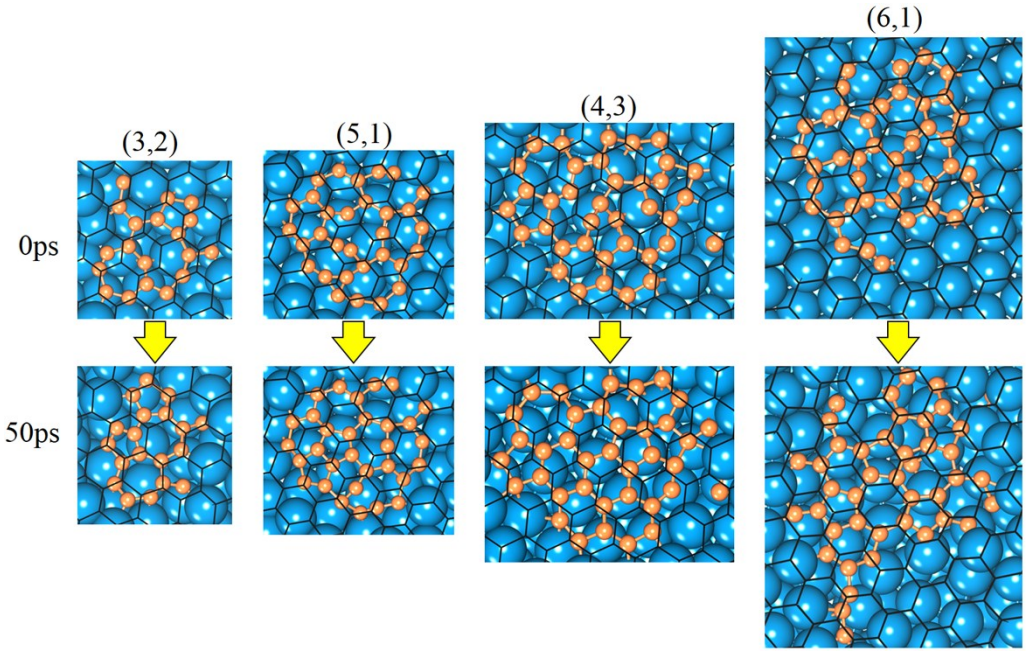

Figure S1. Initial and final C structures on the GTL (3,2), GTL (5,1), GTL (4,3), and GTL (6,1) −covered Ni (111) surface obtained in 50 ps MD simulation at 1000 K, respectively. Cyan spheres represent Ni atoms, black sticks represent GTL and orange spheres represent C atoms for growing the adlayer graphene.

Movie S1. The detailed evolution trajectories of the adlayer defects bonded with GTL(1,1) within the first 10 ps in the MD simulation at 1000K. Cyan spheres represent Ni atoms, grey sticks represent GTL, orange spheres represent C atoms for growing the adlayer graphene, green spheres represent the adlayer defect bonded with GTL(1,1) and red sphere represents the C atom in the GTL(1,1).

Movie S2. The detailed evolution trajectories of the adlayer defects bonded with GTL(3,1) within the first 10 ps in the MD simulation at 1000K. Cyan spheres represent Ni atoms, grey sticks represent GTL, orange spheres represent C atoms for growing the adlayer graphene, green spheres represent the adlayer defect bonded with GTL(3,1) and red sphere represents the C atom in the GTL(3,1).

Movie S3. The detailed evolution trajectories of the adlayer defects bonded with GTL(2,1) within the first 10 ps in the MD simulation at 1000K. Cyan spheres represent Ni atoms, grey sticks represent GTL, orange spheres represent C atoms for growing the adlayer graphene, green spheres represent the adlayer defect bonded with GTL(2,1) and red sphere represents the C atom in the GTL(2,1).