Supporting Information

Anomalous Frictional Behaviors of Ir and Au Tips Sliding on Graphene/Ni(111) Substrate: Density Functional Theory Calculations

Lei Gao,[†] Yuan Ma,[†] Yanmin Liu,[‡] Aisheng Song,[‡] Tianbao Ma,[*,‡] Yuanzhong Hu,[‡] Yanjing Su,[*,†] and Lijie Qiao[†]

[†]Corrosion and Protection Center, Key Laboratory for Environmental Fracture (MOE), University of Science and Technology Beijing, Beijing 100083, China

[‡]State Key Laboratory of Tribology, Tsinghua University, Beijing 100084, China

Corresponding Author: mtb@mail.tsinghua.edu.cn; yjsu@ustb.edu.cn

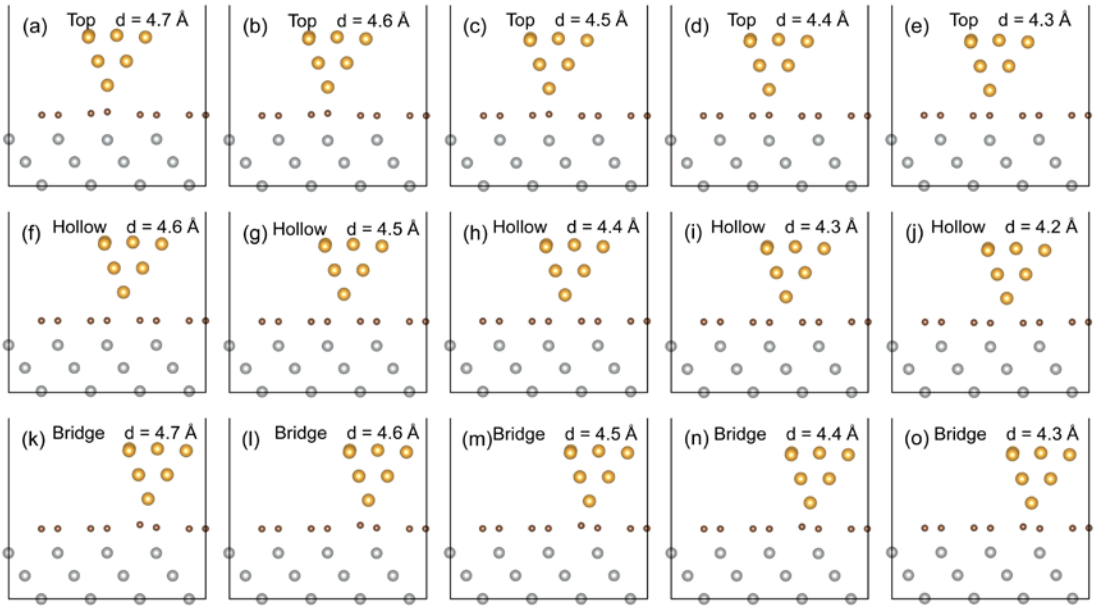

Figure S1. Pushing down process of a 10 atom Au tip on graphene/Ni(111) substrate. (a)−(e) Pushing down on the top site, the distance (between the tip apex atom and the top layer of Ni(111) substrate) d ranges from 4.7 to 4.3 Å; (f)−(j) Pushing down on the hollow site, the distance d ranges from 4.6 to 4.2 Å; (k)−(o) Pushing down on the bridge site, the distance d ranges from 4.7 to 4.3 Å.

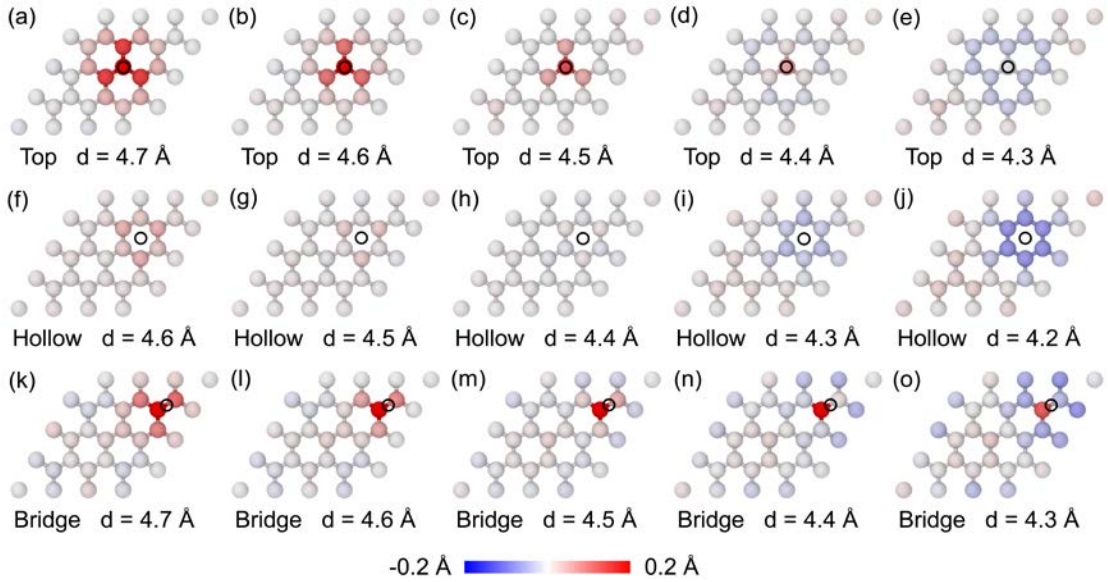

Figure S2. Out-of-plane displacements of C atoms in graphene for the pushing down process of a 10 atom Au tip on graphene/Ni(111) substrate. (a)−(e) Pushing down on the top site; (f)−(j) Pushing down on the hollow site; (k)−(o) Pushing down on the bridge site. The black circle represents the position of the tip apex atom. The red color represents the C atom is attracted

upward and the blue color represents the C atom is pressed downward.

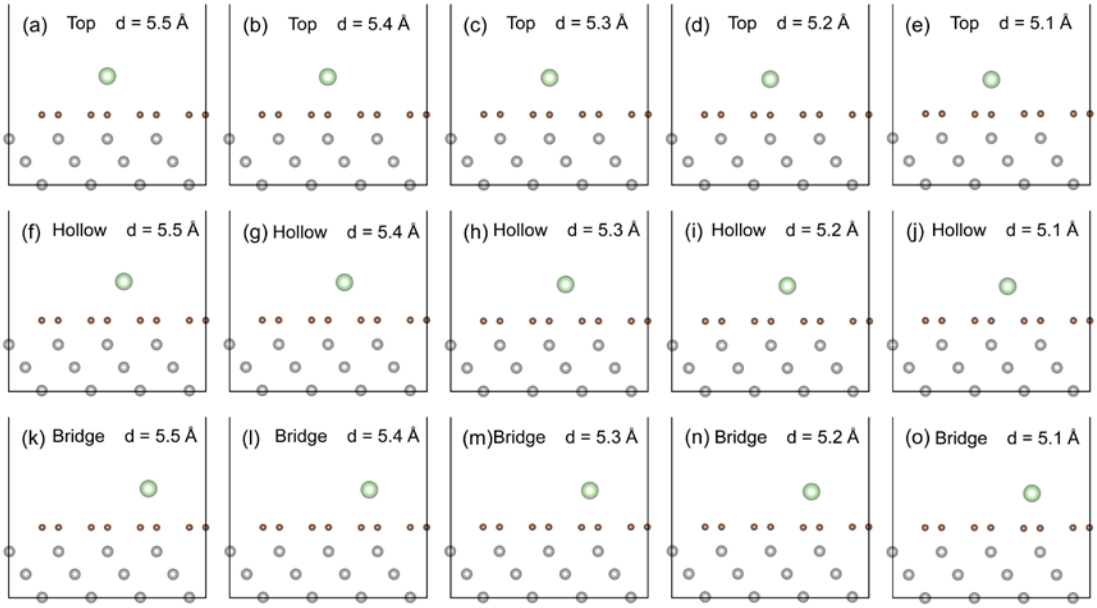

Figure S3. Pushing down process of an Ar atom on graphene/Ni(111) substrate. (a)−(e) Pushing down on the top site, the distance (between the tip apex atom and the top layer of Ni(111) substrate) d ranges from 5.5 to 5.1 Å; (f)−(j) Pushing down on the hollow site, the distance d ranges from 5.5 to 5.1 Å; (k)−(o) Pushing down on the bridge site, the distance d ranges from 5.5 to 5.1 Å.

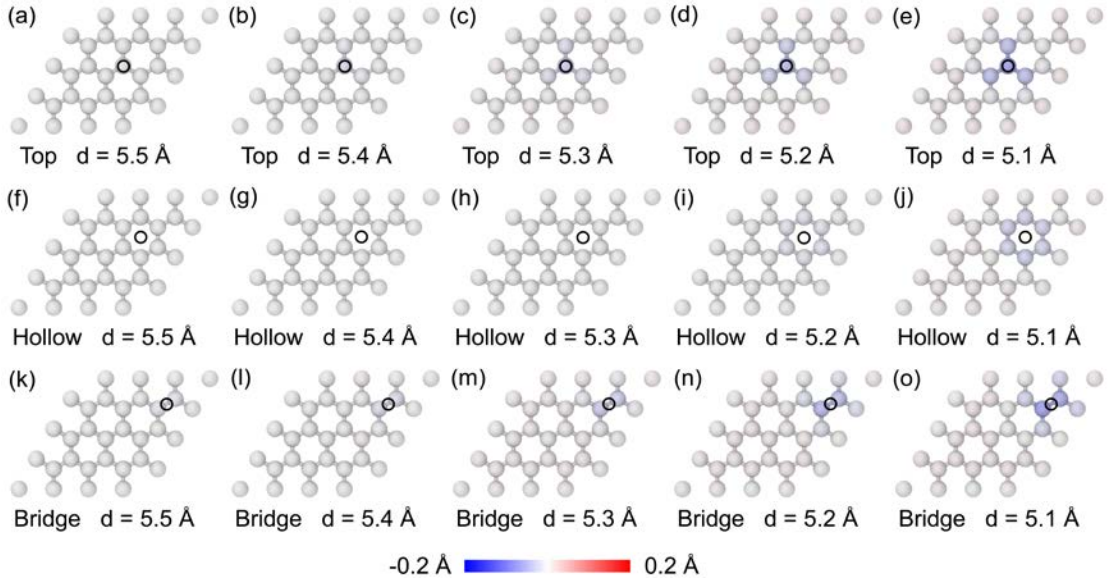

Figure S4. Out-of-plane displacements of C atoms in graphene for the pushing down process of an Ar atom on graphene/Ni(111) substrate. (a)−(e) Pushing down on the top site; (f)−(j) Pushing down on the hollow site; (k)−(o) Pushing down on the bridge site. The black circle represents the

position of the tip apex atom. The red color represents the C atom is attracted upward and the blue color represents the C atom is pressed downward.

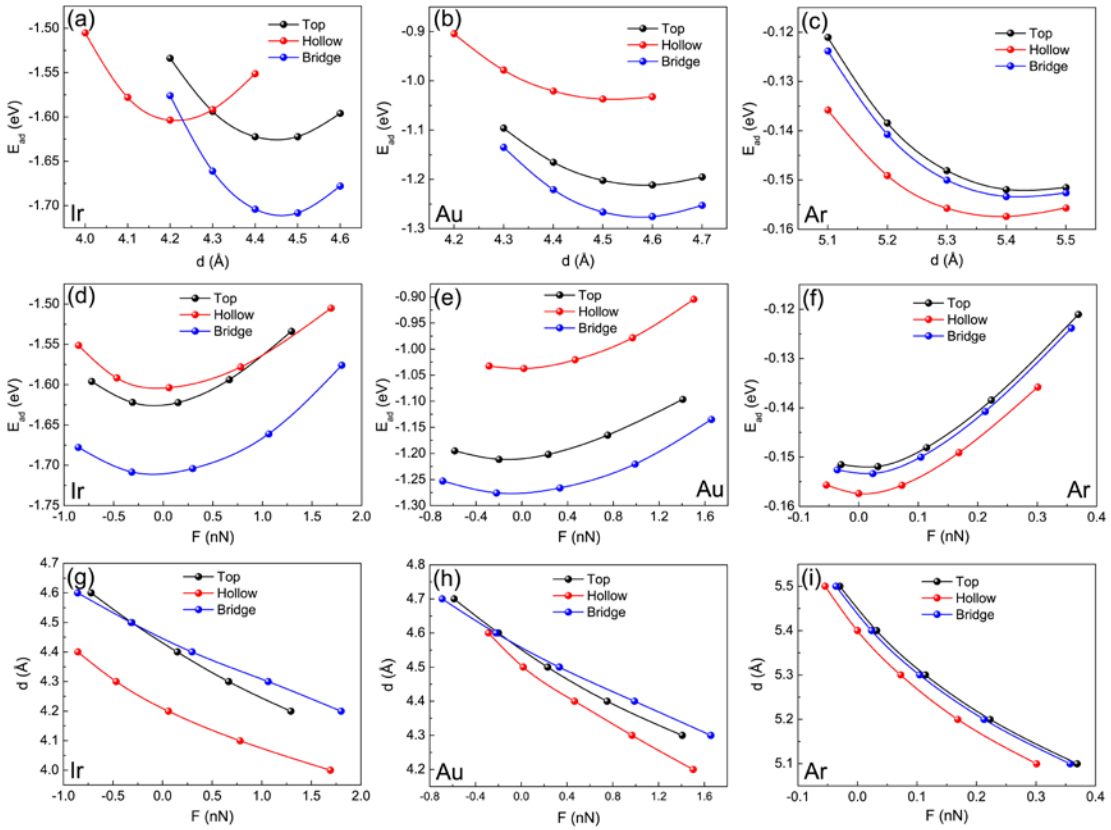

Figure S5. Calculations of the pushing down processes of the 10 atom Ir tip, Au tip, and an Ar atom on the graphene/Ni(111) substrate respectively. (a)−(c) The relationships between the distance d and adsorption energy E_{ad} under the selected normal loads for the Ir tip, Au tip, and an Ar atom respectively; (d)−(f) The adsorption energy E_{ad} under the selected normal loads F for the Ir tip, Au tip, and an Ar atom respectively; (g)−(i) The relationships between the normal load F and distance d under the selected normal loads for the Ir tip, Au tip, and an Ar atom respectively.

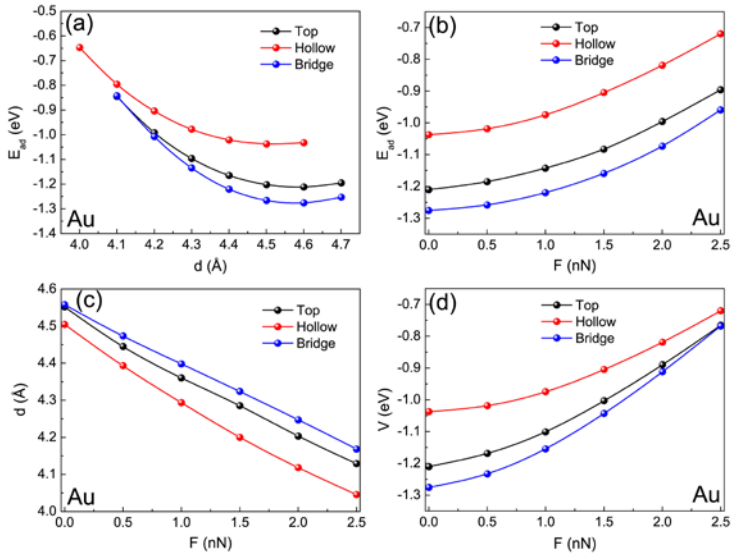

Figure S6. Calculations of the 10 atom Au tip on the graphene/Ni(111) substrate under the normal loads of 0 nN-2.5 nN. (a) The relationship between the distance d and adsorption energy E_{ad}; (b) The adsorption energy E_{ad} under the selected normal loads; (c) The relationship between the normal load F and distance d under the selected normal loads; (d) The potential energy V under the selected normal loads.

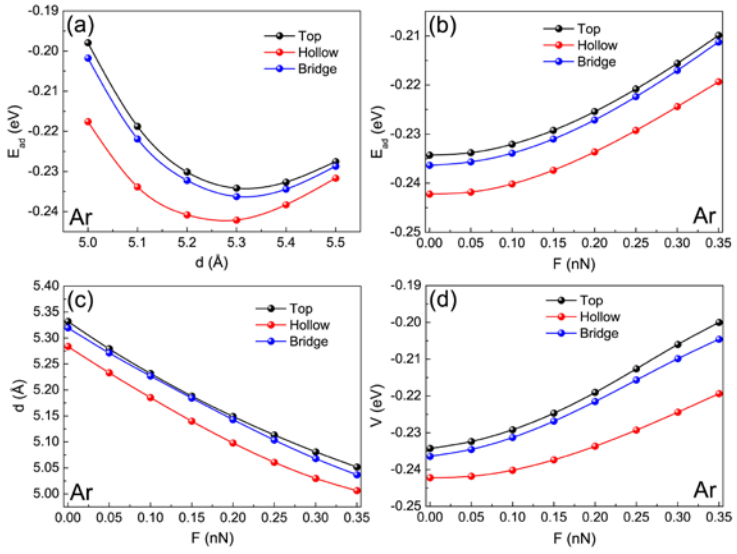

Figure S7. Calculations of the 10 atom Ar tip (the tip was not relaxed) on the graphene/Ni(111) substrate under the normal loads of 0 nN-0.35 nN. (a) The relationship between the distance d and adsorption energy E_{ad}; (b) The adsorption energy E_{ad} under the selected normal loads; (c) The relationship between the normal load F and distance d under the selected normal loads; (d) The potential energy V under the selected normal loads.