Theoretical Studies on the Dynamical Behavior of Atom/Ion Migration on the Surface of Pristine and BN-Doped Graphene

Tong-Kun Zhang [1], Li-Jun Zhou [2],* and Jian-Gang Guo [1],*

[1] Tianjin Key Laboratory of Modern Engineering Mechanics, School of Mechanical Engineering, Tianjin University, Tianjin 300072, China; ztk1173593@163.com

[2] Department of Mechanical Engineering, Tianjin University of Technology and Education, Tianjin 300222, China

* Correspondence: zhoulj_tj@163.com (L.-J.Z.); guojg@tju.edu.cn (J.-G.G.)

Table. S1. The parameters of the dynamical equation [15].

Atom/ion-C	Equilibrium height σ (nm)	Potential well ε (eV)	Mass $m(10^{-26}$kg)
Na^+	0.2935	0.00230	3.819
Li^+	0.2473	0.00433	1.153
Li	0.2374	0.00545	1.153
Mn^{2+}	0.2250	0.00994	9.126
Pt	0.3134	0.00718	32.406