Supporting Information

Hole Defects and Nitrogen Doping in Graphene: Implication for Supercapacitor Applications

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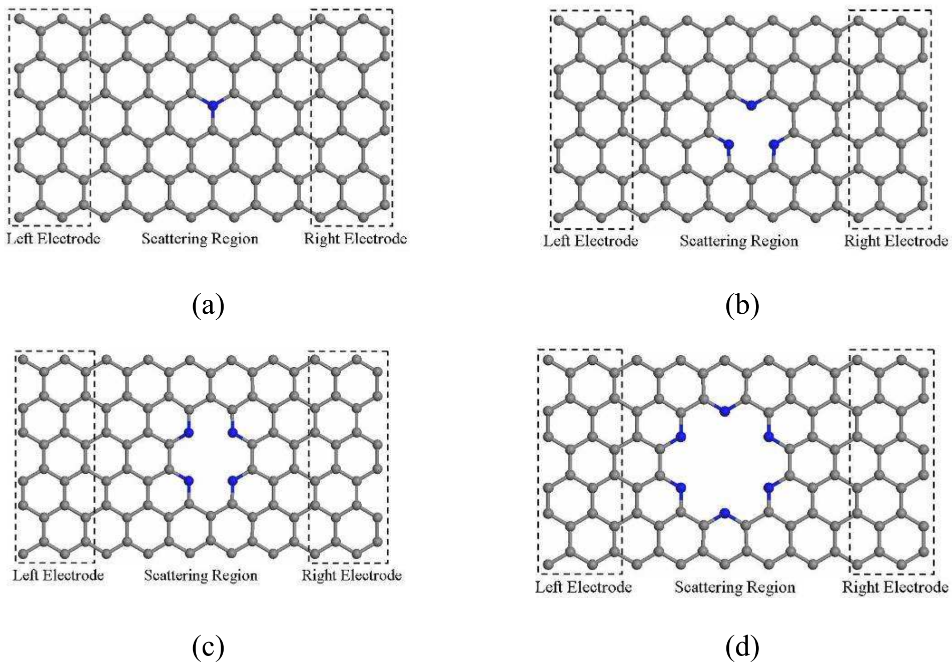

Figure S1 Illustration of the graphene-based devices for transport calculations including left/right electrode and central scattering region: (a) quaternary-like, pyridinic-like with (b) triangular, (c) rectangular, (d) hexagonal hole shapes.

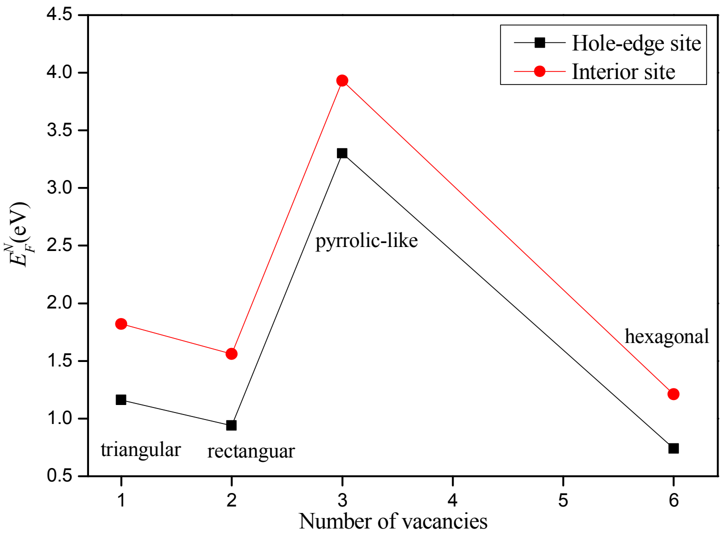

Figure S2 Formation energy of nitrogen doping (E_F^N) for hole edge or interior site with different hole shapes.

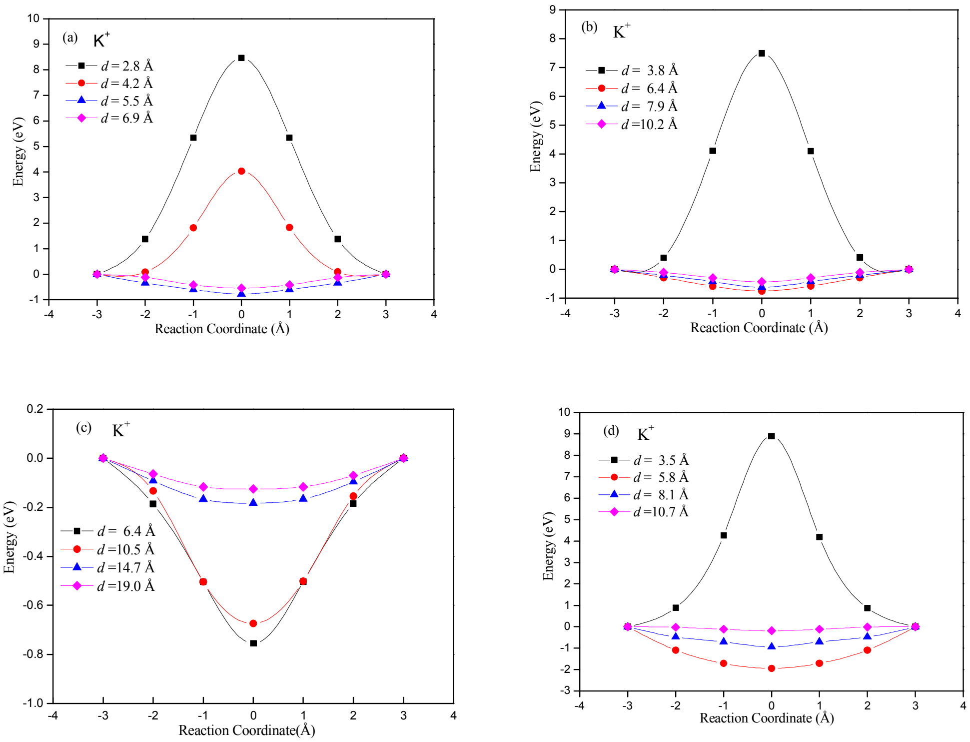

Figure S3 Diffusion barriers for K^+ ions passing through the undoped graphene with different hole sizes: (a) triangular, (b) rectangular, and (c) hexagonal holes for pyridinic-like holes; (d) pyrrolic-like holes.

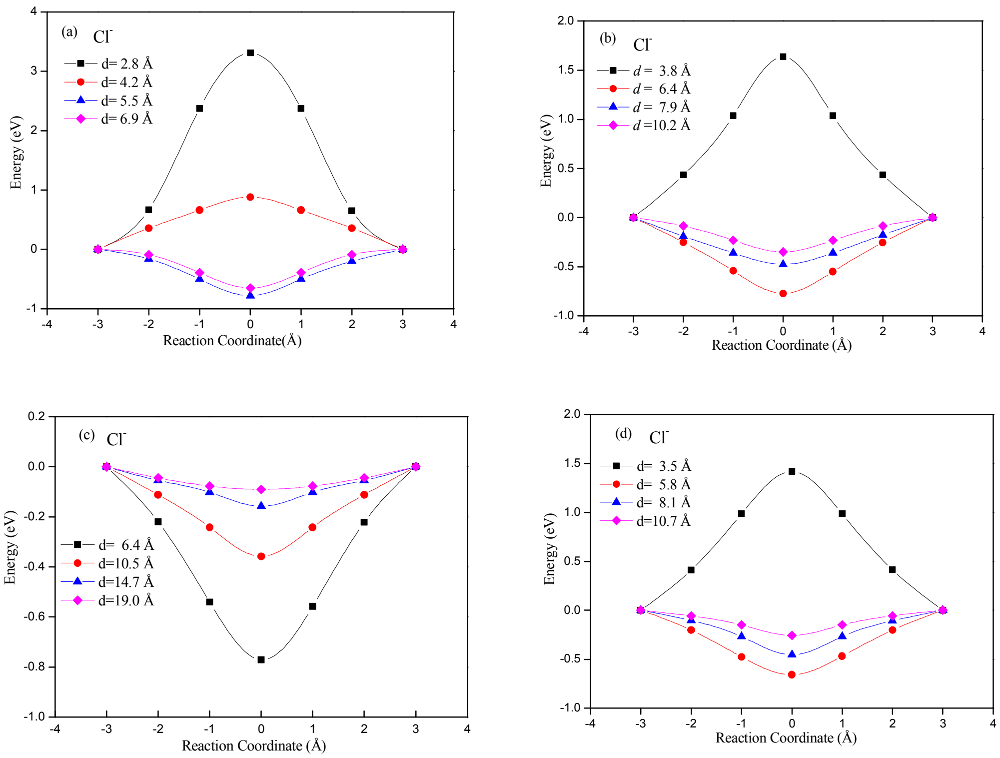

Figure S4 Diffusion barriers for Cl^- ions passing through the undoped graphene with different hole sizes: (a) triangular, (b) rectangular, and (c) hexagonal holes for pyridinic-like holes; (d) pyrrolic-like holes.

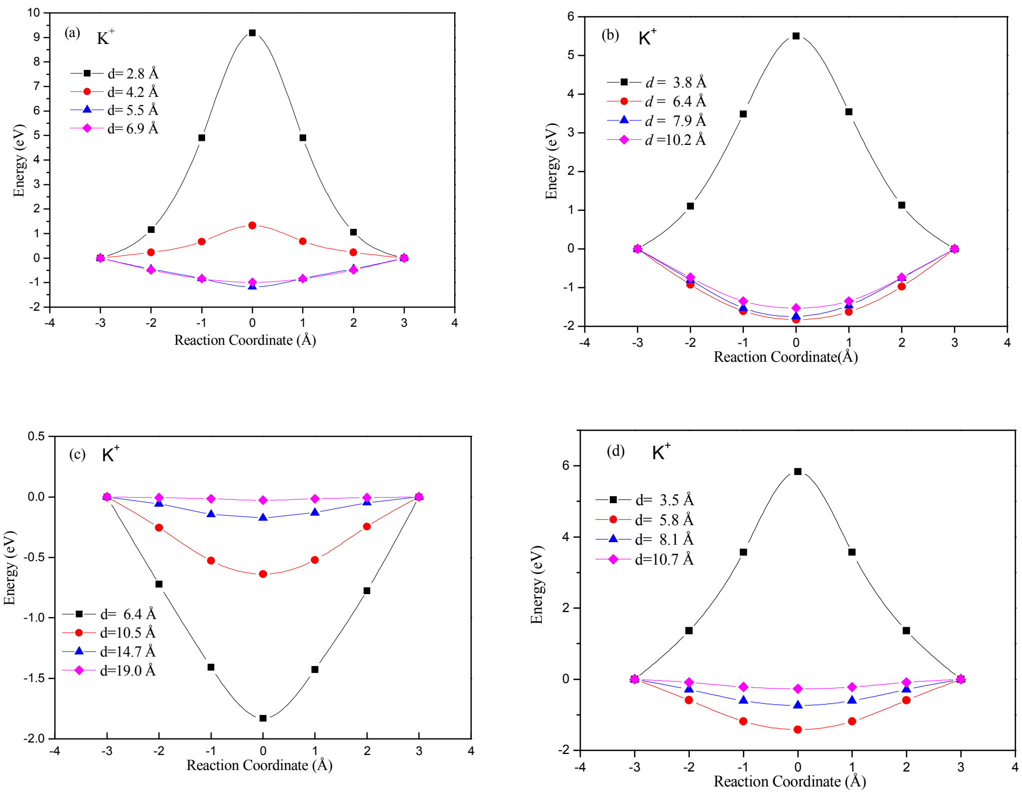

Figure S5 Diffusion barriers for the K^+ ions passing through the N-doped graphene with different hole sizes: (a) triangular, (b) rectangular, and (c) hexagonal holes for pyridinic-like holes; (d) pyrrolic-like holes.

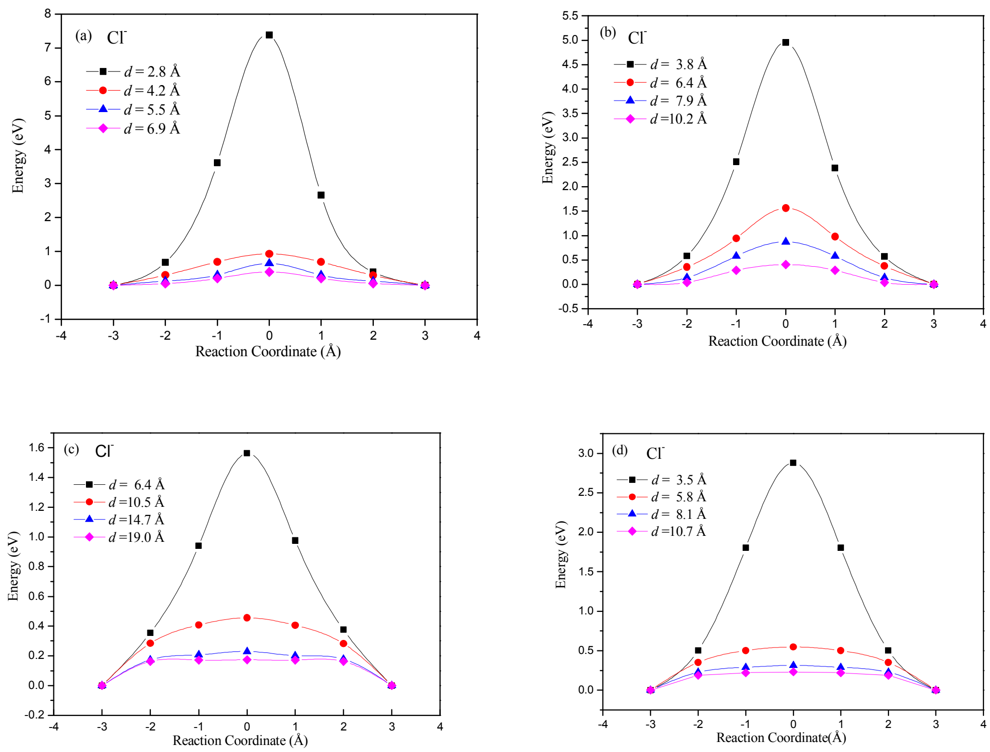

Figure S6 Diffusion barriers for Cl^- ions passing through the N-doped graphene with different hole sizes: (a) triangular, (b) rectangular, and (c) hexagonal holes for pyridinic-like holes; (d) pyrrolic-like holes.

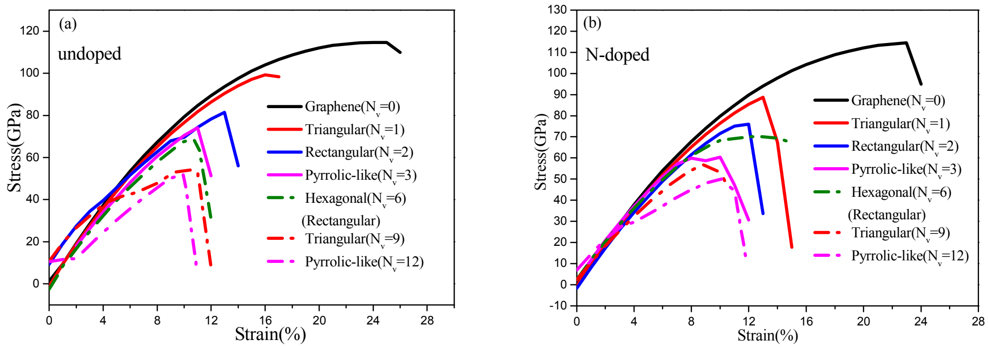

Figure S7 Stress-strain curves of (a) undoped and (b) N-doped graphene sheets. The intrinsic strength is defined as the critical point beyond which the stress decreases with strain.

Table S1. Activation energies (eV) of K^+ and Cl^- ions with different solvent in the N doped hexagonal holes for pyridinic-like systems.

	Vacuum				Acetonitrile (ε = 37.5)				H_2O (ε = 78.54)			
d(Å)	6.4	10.5	14.7	19.0	6.4	10.5	14.7	19.0	6.4	10.5	14.7	19.0
K^+	–1.78	–0.68	–0.23	–0.08	–0.79	–0.16	–0.01	–0.004	–0.77	–0.18	–0.06	–0.002
Cl^-	1.11	0.24	0.07	0.02	1.10	0.20	0.008	0.003	1.11	0.19	0.004	0.02