SUPPORTING INFORMATION

A direct molecular orbital-molecular dynamics (MO-MD) Study on the Diffusion of the Li ion on fluorinated graphene surface

Hiroto TACHIKAWA*

*Division of Materials Chemistry, Graduate School of Engineering, Hokkaido University, Sapporo 060-8628, Japan*

1. Structures of benezene-Li$^+$ complexes

Table S1. Optimized parameters of benzene-Li$^+$ complex. Bond lengths and angles are in A and in degrees, respectively. Notation H (in A) means height of Li+ from benzene ring.

|	R / A	θ / degree	H / A
AM1	2.5673	56.75	2.1471
PM3	2.5561	56.70	2.1365
B3LYP/LANL2MB	2.2452	50.50	1.7326
MP2/6-311++G(d,p)	2.3412	53.03	1.8704
B3LYP/LANL2DZ	2.4175	54.09	1.9580
B3LYP/6-31G(d,p)	2.3162	52.73	1.8433
MP2/6-31G(d)	2.3823	53.82	1.9228
B3LYP/6-31G(d)	2.3481	53.21	1.8805
MP4SDQ/6-311G(d,p)	2.3345	52.92	1.8623
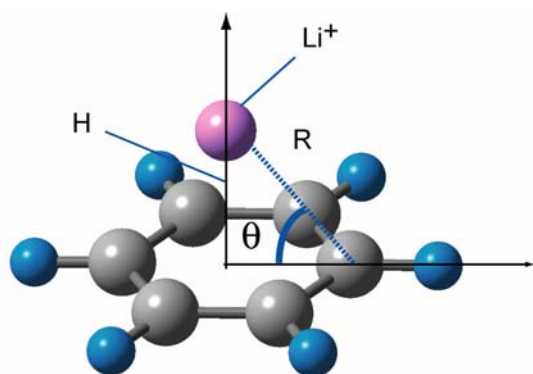
2. Structural relaxation of site D.
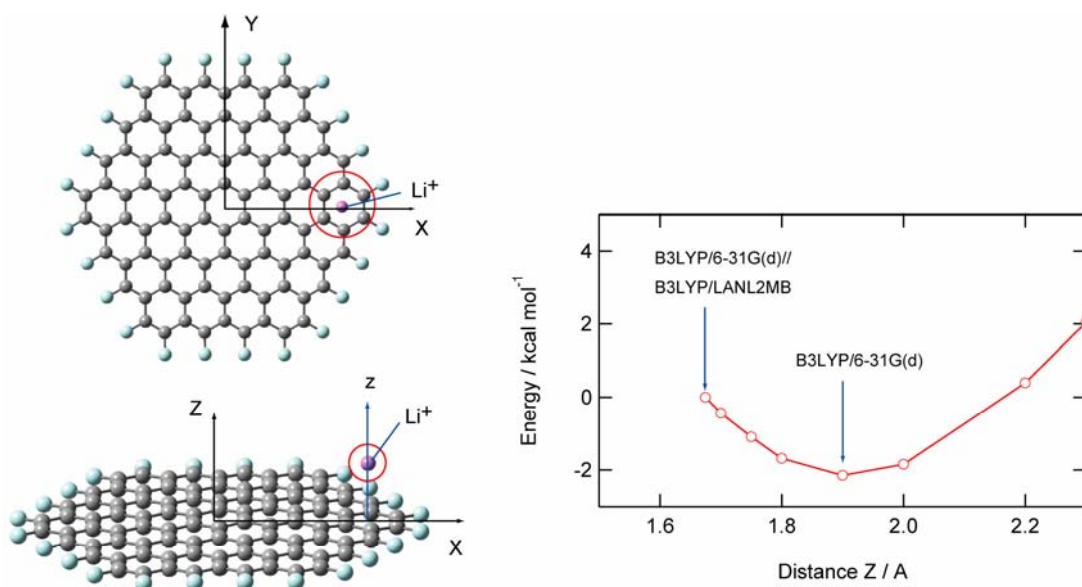
Figure S1. Structure of Li^+ trapped in *site D* and potential energy curve for Li^+ ion plotted as a function of distance Z. True minimum of Li^+ in *site D* is significantly far from the optimized point of B3LYP/LANL2MB level.

3. Potential energy curves relevant for movement of Li^+ along the X axis.
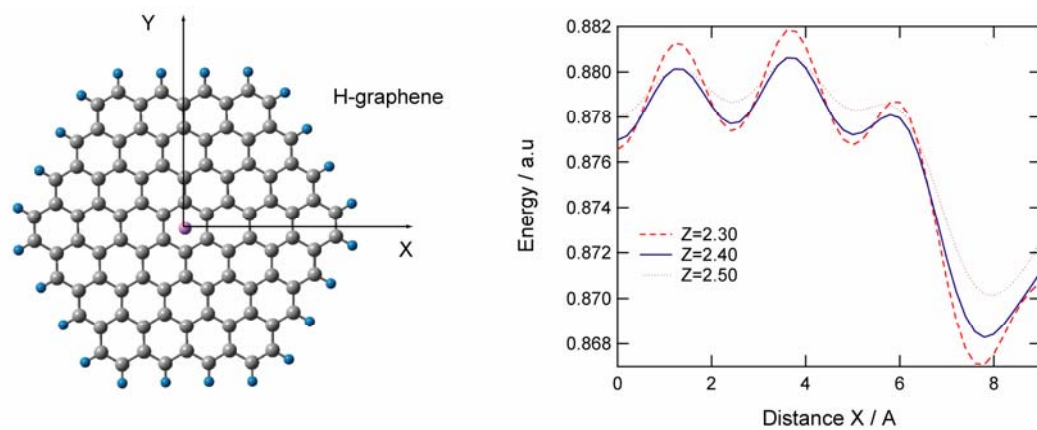
Figure S2. Potential energy curves of Li^+ along the sites A-B-C-D on H-graphene.