

Direct ab-initio MD study on the diffusion of lithium ion on the Nano-Carbon Materials

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Abstract

The diffusion dynamics of the Li⁺ ion on carbon materials such as graphene and fullerene (C₆₀) have been investigated by means of direct molecular orbital-molecular dynamics (MO-MD) method. Simulation temperatures were chosen in the ranges 10-1200 K. The dynamics calculations showed that the diffusion coefficients for the Li⁺ ion on the C₆₀ surface are larger than those of the graphite surface at low temperature (below 300 K). Those of both C₆₀ and graphene surface were almost equivalent at medium temperatures around 300 K. At higher temperatures (T > 300K), the coefficients for graphene surface were significantly larger than those of C₆₀. On the basis of theoretical results, we designed an ion switching molecular device composed of C₆₀ and graphite sheet.

Introduction

Graphite, graphenes, and fullerenes (C₆₀) interact efficiently with several chemical species. In particular, the interaction with alkali ion and atom are important because these species diffuse easily on the surface of these carbon materials [1]. Hence, the character has been applied to the ion carrier material with the performance as high electromotive. However, the diffusion mechanism is not clearly understood. In the present work, diffusion processes of the lithium and sodium ions (Li⁺ and Na⁺) on the graphite, graphenes and C₆₀ are investigated by means of direct molecular orbital-molecular dynamics (MO-MD) method developed by us [2,3]. On the basis of theoretical results, high performance molecular devices are designed.

Method of calculations

Diffusion processes of the Li⁺ ion on the C₆₀ surface were investigated by means of direct molecular orbital-molecular dynamics (MO-MD) method.¹⁷⁻¹⁹ The total energy

and energy gradient on the multi-dimensional potential energy surface were calculated at each time step at the AM1-MO level of theory, and then classical equation of motion is full-dimensionally solved. Therefore, charges and electronic states of the Li ion and all carbon atoms are exactly treated within the level of theory at each time step. This point is much different from usual classical molecular dynamics (MD) calculation where the charges of all atoms and ion are constant during the diffusion. Hence, one can obtain details of the diffusion processes of lithium ion on amorphous carbon using direct MO-MD method.

Results and discussion

Arrhenius plots of the diffusion coefficients of lithium ion on graphite and C₆₀ are given in Figure 1. At low temperature below 200 K, the diffusion coefficient on C₆₀ is significantly larger than that on graphite. At intermediate temperature, the coefficients for both surfaces are equivalent each other. On the other hand, the coefficient on the graphite becomes larger at higher temperatures. On the basis of these results, a new molecular device is designed.

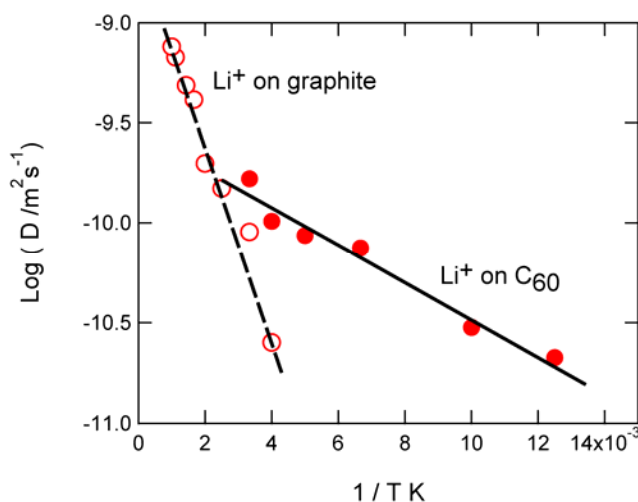


Figure 1. Arrhenius plots of diffusion coefficients of lithium ion on the graphene and C₆₀ surfaces calculated by means of direct molecular orbital-molecular dynamics (MO-MD) method.

References

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