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Confined Li ion migration in the Silicon-Graphene complex system:

An ab initio investigation

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Highlights

- Li ion migration property of Silicon-Graphene complex systems are investigated.
- The effects of graphene coating on the migration of Li ions are discussed in detail.
- The activation energy is as low as 0.028 eV for Li ions migration in the Si-Gr system.
- Through AIMD calculations, it is found that the graphene coating can improve Li migration.

Abstract

Silicon-Carbon complex systems play an important role in enhancing the performance of Si-based anode materials for Li ion batteries (LIBs). In this work, the Li migration property of the Silicon-Graphene (Si-Gr) complex systems are investigated by using first-principles calculations. Especially, the effects of graphene coating on the migration of Li ions are discussed in detail. The distance between Si surface and graphene in the Si-Gr system significantly affects the lateral migration of Li ions. With the decrease of the distance from 4.715 to 3.844 Å, the energy barrier of Li ion migration also decreases from 0.115 to 0.067 eV, which are all lower than that of the case without graphene. However, smaller distance (3.586 Å) brings the high energy barrier (0.237 eV). Through AIMD calculations, it is found that the graphene coating in the Si-Gr complex system would result in the larger intercalation depths,

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