Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for

Li deposition and desolvation with electron transfer at a silicon/propylene-carbonate interface: Transition-state and free-energy profiles by large scale first-principles molecular dynamic

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Movie of the desolvation process shown in Fig. 3 in the main text is in file "desolvation.mpg."

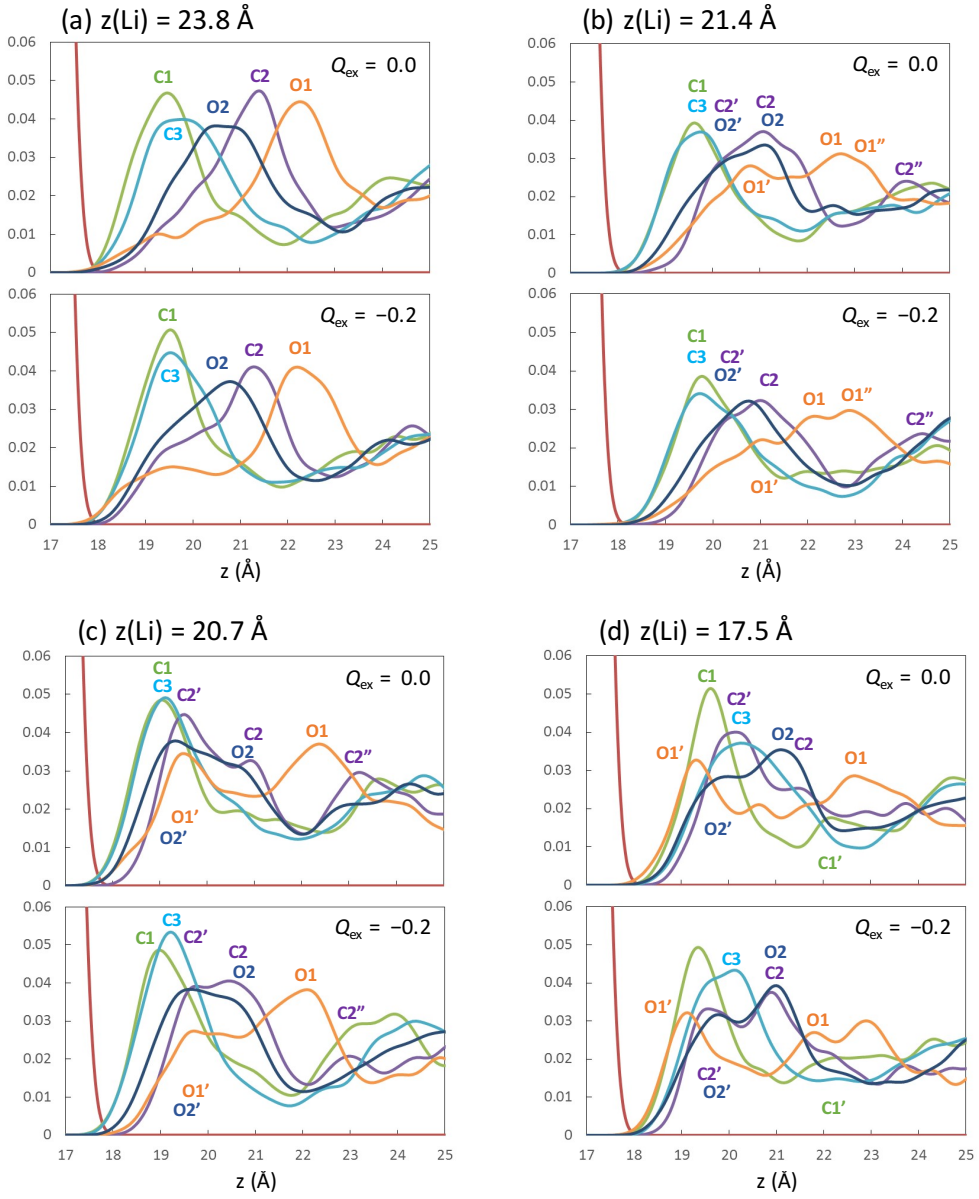

Figure S1 Atom distributions of PC molecules along the z-axis for different positions of Li (z(Li)) and excess charges (Q_{ex}). Regarding atom indexes in the figures, refer to Fig. 3(a).

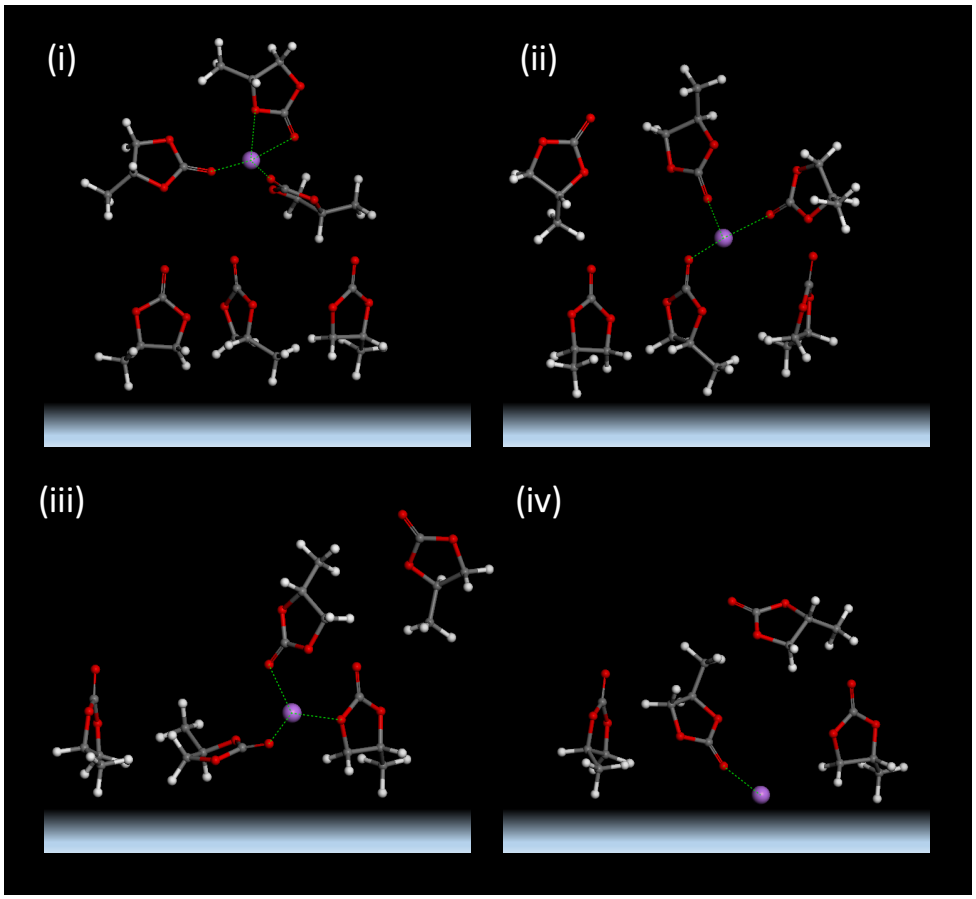

Figure S2 Schematic configurations of PC molecules during desolvation at the different Li position near Si-electrode surface. (i) The Li ion in the bulk region is solvated by three PC molecules through O1. (ii) Exchange of the solvation molecule takes place between the molecule in the bulk and that in the PC-molecular layer, keeping the same solvation structure through O1. (iii) The Li ion goes through the PC-molecular layer pushing down one of PC molecules in the layer (transition state), giving the different solvation structure through O1 and O2. (iv) The number of solvation PC molecules decreases during Li deposition on the Si surface.

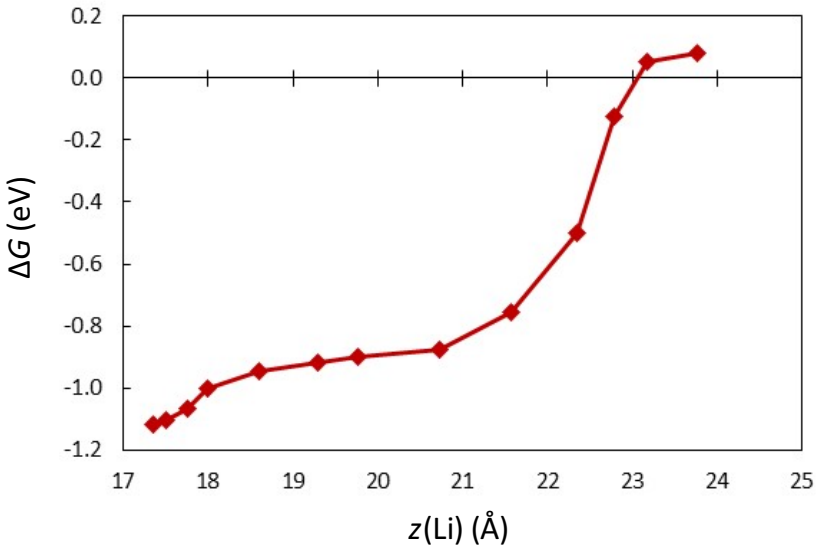

Figure S3 Free-energy difference (ΔG) for Li-deposition process with different excess charges Q_{ex}. $\Delta G = E(Q_{ex}{=}{-}0.20\mathrm{e}) - E(Q_{ex}{=}0)$