

# Microscopic Origin of the SEI Formation Difference Between in *Cis*- and in *Trans*-2,3-Butylene Carbonate Based Electrolyte

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**Introduction** Solid electrolyte interphase (SEI), which consists of reduction reaction products of electrolyte, is closely related to the lifetime and safety of Li-ion battery. Two cyclic carbonates, *cis*- and *trans*-2,3-butylene carbonate (*c/t*-BC), are mutually geometric isomers, and thus their characteristics are almost the same, e.g., dipole moments, energy levels of the highest occupied molecular orbital, and the lowest unoccupied molecular orbital. Furthermore, reduction products of *c*- and *t*-BC are identical after their ring-opening reaction [1]. However, it was reported that *t*-BC-based electrolyte enables the reversible reaction of graphite anodes [as in ethylene carbonate (EC)], while *c*-BC-based one causes the exfoliation of graphite [as in propylene carbonate (PC)] [1]. To understand its microscopic origin of the different electrochemical behavior of *t*-BC and *c*-BC, we have tried to clarify microscopically the SEI formation by Red Moon (RM) simulation [2,3].

**Method** Interface models of electrolyte and carbon anode are prepared assuming essential elementary chemical reactions of SEI formation (shown in the figure). A number of RM simulations of SEI formation were performed in 1M LiPF<sub>6</sub>/*c*- or *t*-BC-based electrolytes.

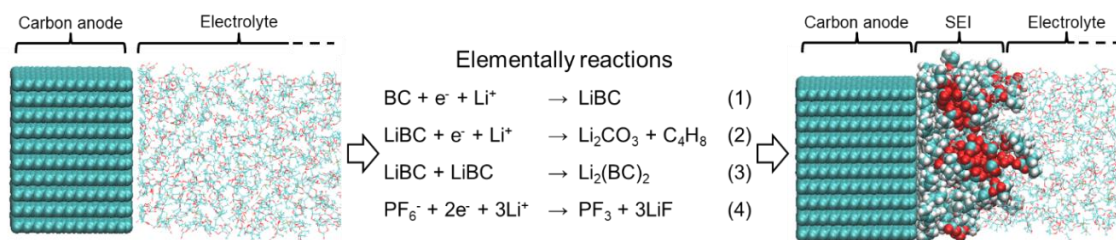


Figure. Simulation system in 1M LiPF<sub>6</sub>/*t*-BC and a list of elementary chemical reactions. Anode and SEI are illustrated with balls while the electrolyte with sticks.

**Results and discussion** A typical snapshot of SEI is shown in the figure. We found a difference in the composition of SEI components, namely, the SEI produced in *c*-BC-based electrolyte contains less organic compounds [LiBC, Li<sub>2</sub>(BC)<sub>2</sub>] than that in *t*-BC-based one. Note that the previous theoretical study of PC and EC showed that the SEI in PC-based electrolyte, which causes exfoliation of graphite, contains less organic compounds than that in EC [3]. From this perspective, less number of organic compounds in *c*-BC can cause instability of the SEI as in PC. According to the further analyses, the strong solvation of “LiBC” in *c*-BC-based electrolyte suppresses the contact between “LiBC” in the elementary reaction (3), which results in the decrease of organic compounds. It is concluded, therefore, that such a small geometrical difference between *c*-BC and *t*-BC leads to the large difference in the SEI formation. This theoretical study suggests that the solvation effect to the intermediate species is one important key to make a stable SEI.

## References:

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