Supporting Information for
Quantum Chemistry Study of the Oxidation-Induced Stability and Decomposition of Propylene Carbonate-Containing Clusters

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The oxidation potential of PC₂ has been calculated by using B3LYP and G4MP2 method respectively as is shown in Figure S1. It can be found the results from B3LYP are in good agreement with G4MP2.

![B3LYP and G4MP2](image)

Figure S1. Optimized structures and calculated oxidation potentials (vs. Li/Li⁺) of PC₂, using B3LYP/6-311++G(d) and G4MP2 method respectively.

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