Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

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 PC_2 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.

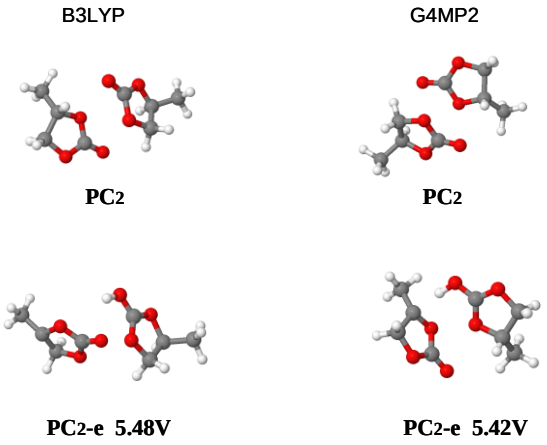

Figure S1. Optimized structures and calculated oxidation potentials (vs. Li/Li^+) of PC_2, using B3LYP/6-311++G(d) and G4MP2 method respectively.

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