Supplemental Information

Atomic-Level Investigation on the Oxidation Efficiency and Corrosion Resistance of Lithium Enhanced by the Addition of Two Dimensional Materials

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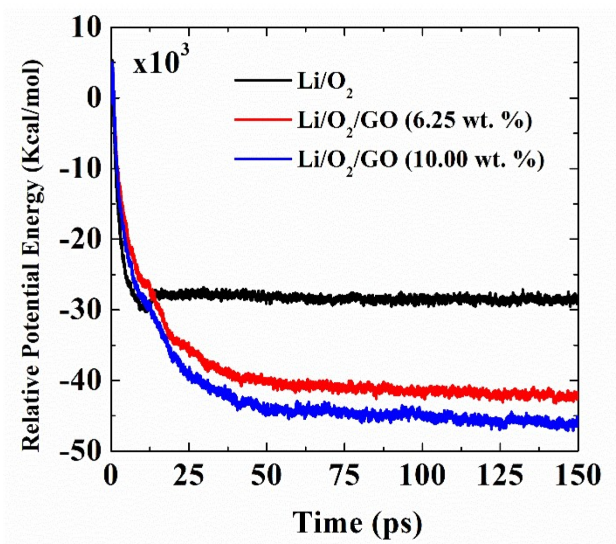

Figure S1. Variations of the relative potential energy of Li for different concentrations of GO as a function of time

We varied the concentration of GO in the system, focusing on two concentrations of 6.25 wt. % and 10 wt. %, as depicted in Fig. S1. It can be noted that when the concentration of GO in the system is increased from 6.25 wt. % to 10 wt. %, the relative potential energy of bare Li reduced notably. Therefore, it can be inferred that raising the concentration of GO greatly improves the system's oxidation efficiency. This reason can be explained form collision and rate laws. According to the Collision Theory, the frequency of collisions between two reactants increases with the concentration of reactants. While the concentration of GO in the system was increased, the number of Li-H bonds rose as well, assisting in reducing the potential energy of bare Li and therefore enhancing the rate of oxidation. Further, the amount of O-containing functional groups, such as carboxyl (-COOH), hydroxyl (-OH), carbonyl (-C=O), epoxy (C-O-C), and ketone (-C=O), was enhanced, resulting in a higher oxidation rate as the concentration of GO has been increased.

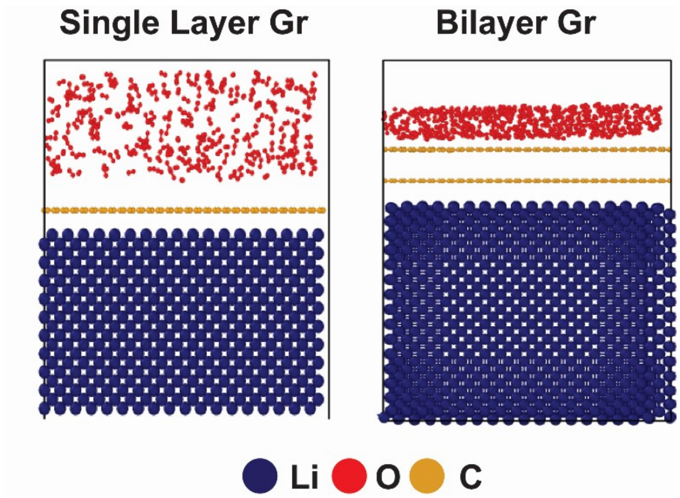

Figure S2. Initial coordinates of the Li/O_2/Gr system. Note, both single and bilayer Gr has been taken into account.

We further varied the number of Gr sheets in the system and recorded the Li-O bond with time, which is summarized below. It is worth noting that just a single layer of Gr sheet is sufficient to prevent Li from oxidation entirely.

Table S1. The bond population of Li-O for different numbers of Gr sheet as a function of time

No. of Gr layer	No of Li-O bonds at time = 75 ps	No of Li-O bonds at time = 150 ps
Single	0	0
Double	0	0