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Supporting Information

Monolayer Graphitic Germanium Carbide (g-GeC): The Promising Cathode Catalysts for Fuel Cell and Lithium-Oxygen Battery Applications

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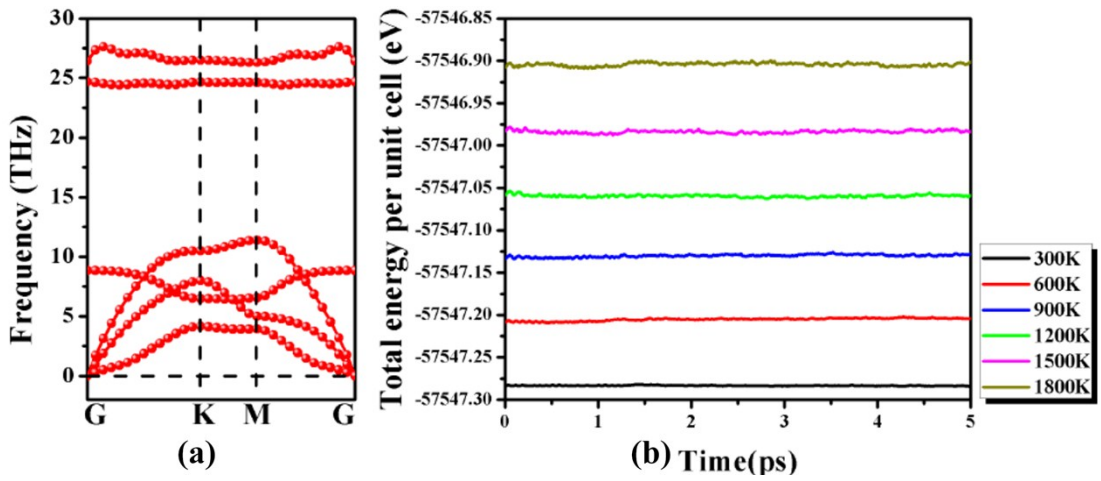

Figure S1. (a) The phonon spectrum of 2D monolayer g-GeC and (b) the trajectories of ab initio molecular dynamics at 300~1800 K.

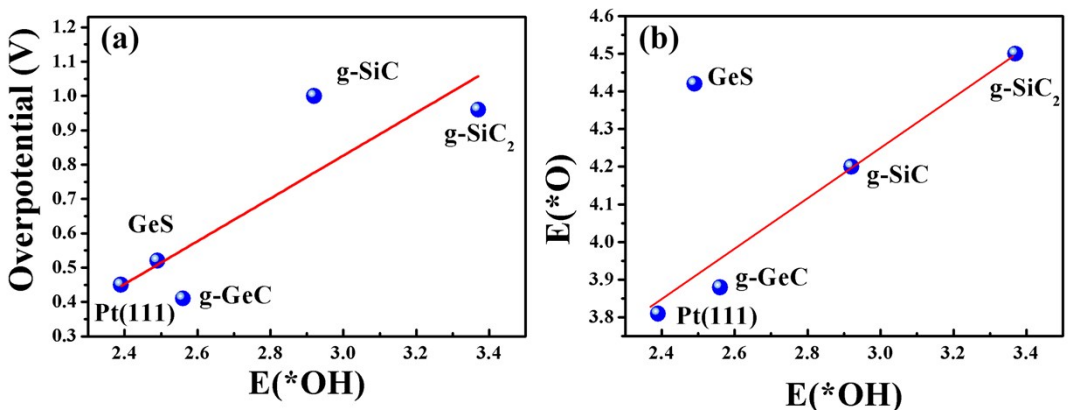

Figure S2. Trends in the calculated overpotential in the acid environment and the binding energy of *O plotted as a function of the *OH binding energy.

Table S1. The comparison of Gibbs free energy in the formation of $*Li_3O_2$, $*Li_2O_4$, $*Li_4O_2$ and $*Li_3O_4$.

$G(*Li_3O_2+O_2+(Li^++e^-))-G(*Li_2O_4+2(Li^++e^-))=-2.26$ eV
$G(*Li_4O_2+O_2)-G(*Li_3O_4+(Li^++e^-))=-1.94$ eV