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First-Principles Density Functional Theory Modeling Study on the Redox Chemistry of Graphene Oxides Affected by Placement Geometry of Oxygen Functional Groups SUNGHEE KIM, KI CHUL KIM, SEUNG WOO LEE, SEUNG SOON JANG, Georgia Inst of Tech — To date, lithium-ion batteries have been extensively gained attention due to their promising potential in the industry. Despite their promising properties, improving their poor power density is still needed for practical applications. In addition, sustaining the high redox potential in the lithium-ion batteries is prerequisite for exhibiting the high energy and power densities. Recently, layered carbon materials including graphenes and carbon nanotubes have been paid special attention as promising electrode candidates with high power densities due to their exceptionally high surface area and active oxygen functional groups on their surfaces. However, the lack of reliable information on the redox chemistry of the candidates is the obstacle to be uncovered for practical applications. In this study, we investigated the redox chemistry of graphene oxides cluster models with well-controlled hydroxyl functional groups at the edge. First-principles density functional theory approach was employed to understand the geometric effect of the incorporated hydroxyl functional groups on the redox chemistry. Our study will provide an insight on the strategy for improving the redox potentials of graphene-based electrode candidates.

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