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Quinone Derivatives for Lithium-Ion Batteries: First-Principles Density Functional Theory Modeling SEUNG SOON JANG, KI CHUL KIM, School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA 30332-0245, USA, TIANYUAN LIU, SEUNG WOO LEE, G. W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA 30332-0405, USA — The Li binding thermodynamics and redox potentials of seven different quinone derivatives are investigated as positive electrode candidates for lithium-ion batteries. First, using the density functional theory (DFT) calculations on the interactions between the quinone derivatives and Li ions, it is found that Li ions are dominantly bound with carbonyl groups of the molecules. Second, it is revealed that the redox chemistry of the quinone derivatives can be tuned by the modification of their chemical structures. Further DFT-based investigations on the redox potentials of the Li-bound quinone derivatives provide an insight on the change in their redox chemistry during the discharging processes. The redox potential and charge capacity are improved by modifying the quinone derivatives with electron-withdrawing carboxylic groups. Through this study, it is also found that the cathodic activity of a quinone derivative during the discharging processes strongly relies on the solvation free energy effect as well as the number of available carbonyl groups for further Li binding. To the best of our knowledge, the changes in the redox potential of the redox-active molecules during the discharging processes is reported for the first time.

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