Supporting Information

Key features of organic electrolyte molecules in lithium ion battery

Takao Tsuneda,1* and Yoshitaka Tateyama2,3
1Graduate School of Science, Technology, and Innovation, Kobe University, Kobe 657-8501, Japan
2Global Research Center for Environment and Energy based on Nanomaterials Science (GREEN), National Institute for Materials Science (NIMS), 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan
3Center for Materials Research by Information Integration (CMI2), Research and Services Division of Materials Data and Integrated System (MaDIS), National Institute for Materials Science (NIMS), 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan

* Corresponding author: tsuneda@phoenix.kobe-u.ac.jp
Fig. S1. The images of the optimum geometries of lithium complexes with 14 types of ten organic electrolyte molecules. The coordination numbers of the optimum complexes, four-coordination (4-c) and five-coordination (5-c), are shown for neutrals (n) and cations (c). The viscosity is also shown in centipoise (cP).
Fig. S2. The molecular orbital images of the LUMOs of the monovalent cations and the SOMOs of the neutrals for lithium complexes with 14 types of ten organic electrolyte molecules. For EC and PC, the HOMOs of the monovalent cations and the LUMOs of the neutrals are also shown.