Abstract Submitted
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***Ab inito* molecular-dynamics study of EC decomposition process on Li_2O_2 surfaces** YASUNOBU ANDO[1], Department of Materials Engineering, The University of Tokyo, TAMIO IKESHOJI, MINORU OTANI[2], Nanosystem Research Institute, AIST — We have simulated electrochemical reactions of the EC molecule decomposition on Li_2O_2 substrate by *ab initio* molecular dynamics combined with the effective screening medium method. EC molecules adsorb onto the peroxide spontaneously. We find through the analysis of density of states that the adsorption state is stabilized by hybridization of the *sp2* orbital and the surface states of the Li_2O_2. After adsorption, EC ring opens, which leads to the decomposition of the peroxide and the formation of a carboxy group. This kind of alkyl carbonates formed on the Li_2O_2 substrate was found in experiments actually

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