Supporting Information

Quantum chemical approach for highly durable anion exchange groups in solid-state alkaline fuel cells

K. Matsuyama[a], H. Ohashi[a], S. Miyanishi[a], H. Ushiyama[b] and T. Yamaguchi*[a]

a. Chemical Resources Laboratory, Tokyo Institute of Technology, R1-17 4259 Nagatsuta-cho, Midori-ku, Yokohama, Kanagawa 226-8503, Japan.
b. Department of Chemical System Engineering, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan.

*E-mail: yamag@res.titech.ac.jp; Tel: +81-45-925-5254; Fax: +81-45-924-5253

The alkaline durability of model molecules were also tested at 120 °C by Monhanty et al. The test condition was shown in the main text. Fig. S1 shows the structure of the model molecules and their LUMO isosurfaces. The relationship between the degradation rate of the model molecules at 120 °C and LUMO of various model molecules is shown in Fig. S2. Their LUMO energies have proximate values from –0.2 to –0.7 eV. Moreover, except for TMHA (10), their LUMO isosurface shapes are also similar. LUMO dependence on the degradation rate could not be confirmed. This could be because other factors such as steric or solvation effects become dominant in such harsh circumstances, which caused the difference of their degradation rates.

Nevertheless, the significance of this research is not diminished. It is not searching for the most durable anion exchange group but searching for rules to find unstable anion exchange groups (such as low LUMO energy and/or π-type LUMO localized on anion exchange groups). By applying such rules, unstable anion exchange groups can be removed in the first design phase, which will be helpful for saving time and cost to successive synthesis phase.

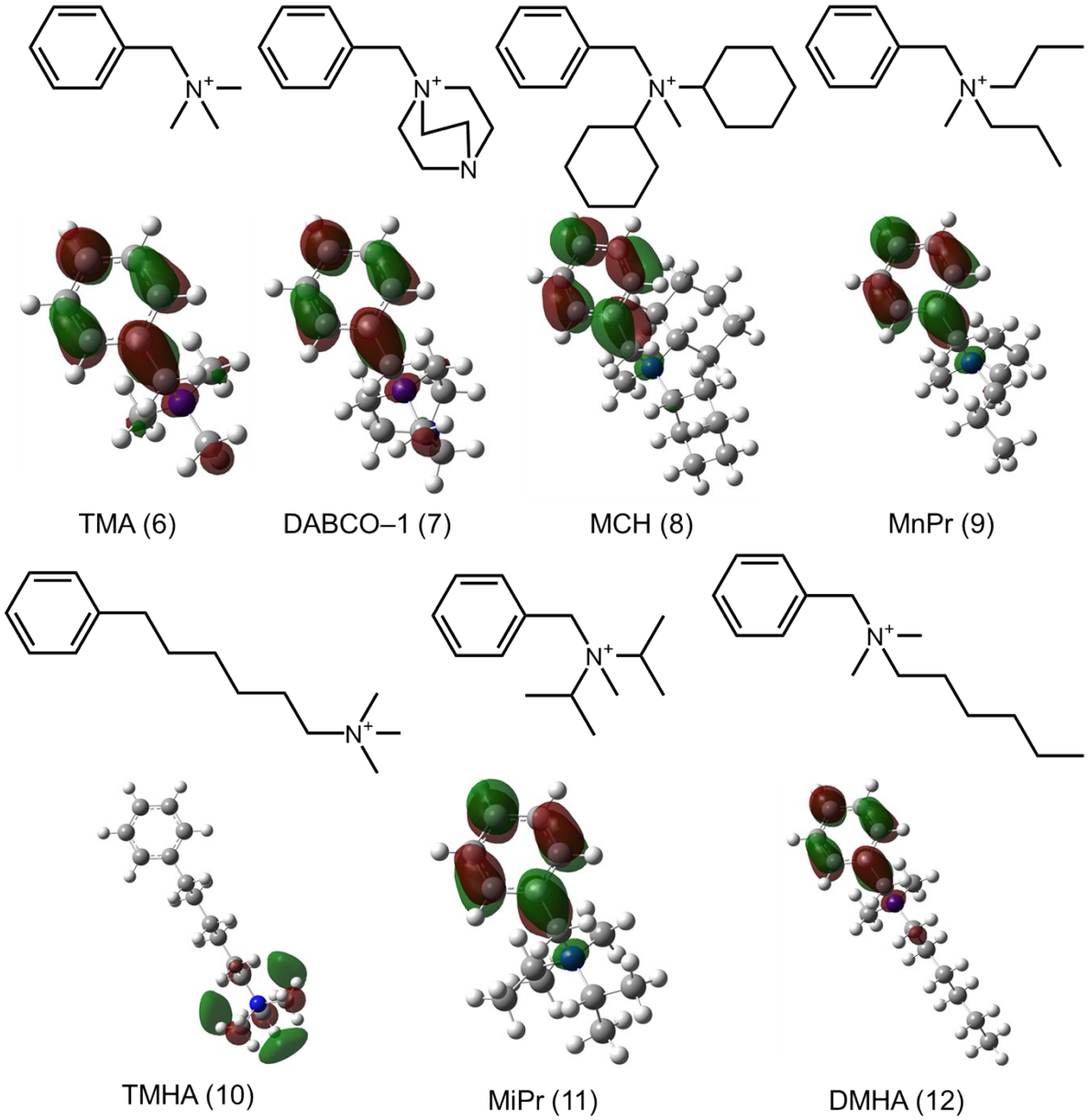

Fig. S1. Molecular structures and LUMO isosurfaces of model molecules (isovalue, 0.04). The model molecules were subjected to decomposition tests at 120 °C.

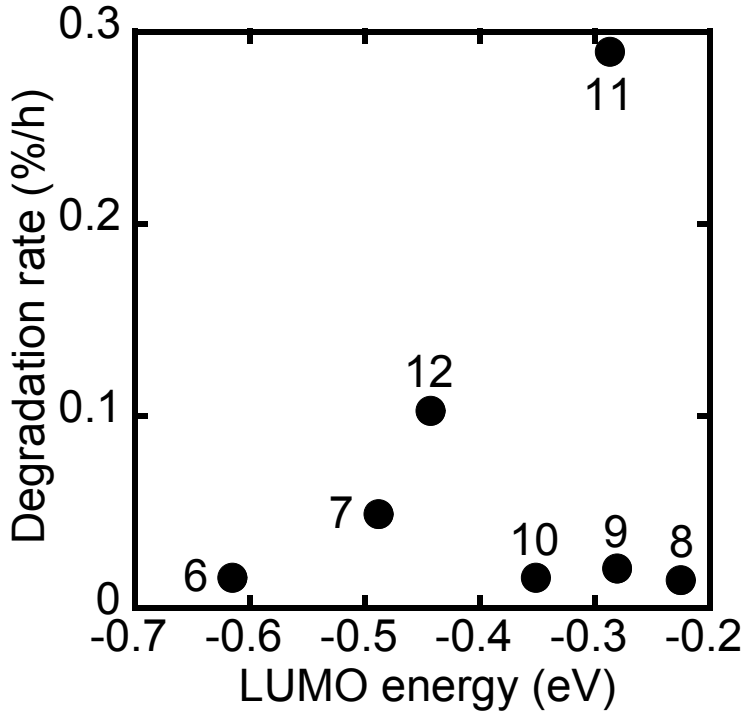

Fig. S2. The relationship between degradation rate at 120 °C and LUMO energy of the model molecules shown in Fig. S1.