Development of High-performance Perfluoro Polymer Electret

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Electret is a dielectric with quasi-permanent charge. The charges trapped in proper electret materials can be stably stored and able to generate an external electrostatic field for tens of years. In recent years, a vibration-driven electret energy harvester attracts much attention, because it can convert ambient low-frequency vibration into electricity. High-performance electret materials have been desired, since the maximum power output of electret energy harvester is proportional to the electret surface potential squared [1]. Also, long-term stability of trapped charge determines the lifespan of the device. Although high-performance electrets have been reported in recent years [2], they are discovered from experimental trials, while its properties were unpredicted. In order to develop a new high-performance electret, it is necessary to understand underlying physics.

In the present study, we made numerical simulations to understand electron trapping phenomenon in polymer electrets using quantum mechanical analysis. An amorphous polymer electret CYTOP (AGC Co., Ltd) is mainly assumed, focusing on the electron trap site and the trap energy for different end groups.

Density functional theory with long-range correction (LC-DFT) calculation is adopted to analyze the electronic state of CYTOP molecules. The LC-BLYP density functional is used to solve Kohn-Sham equation with 6-31+g* basis sets. Three types of CYTOP with different end group are studied as shown in Fig. 1; CTL-S has trifluoromethyl end, CTL-A has carboxyl end, and CTL-M has amidosyl end. Conventionally-used bulk polymer electrets (PE, ETFE, PTFE) are also analyzed for comparison. Fig. 2 shows distribution of electrons trapped in electret tetramers. The electron trapped in PE does not lie on the structure, showing the molecule is electrophobic. On the other hand, clear electrophilicity can be found in fluorine-rich part of ETFE and PTFE. For CYTOP molecules, the trapped electron populates near

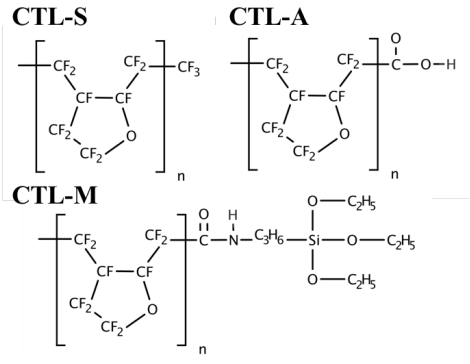

Fig 1. Chemical structure of CYTOP polymers

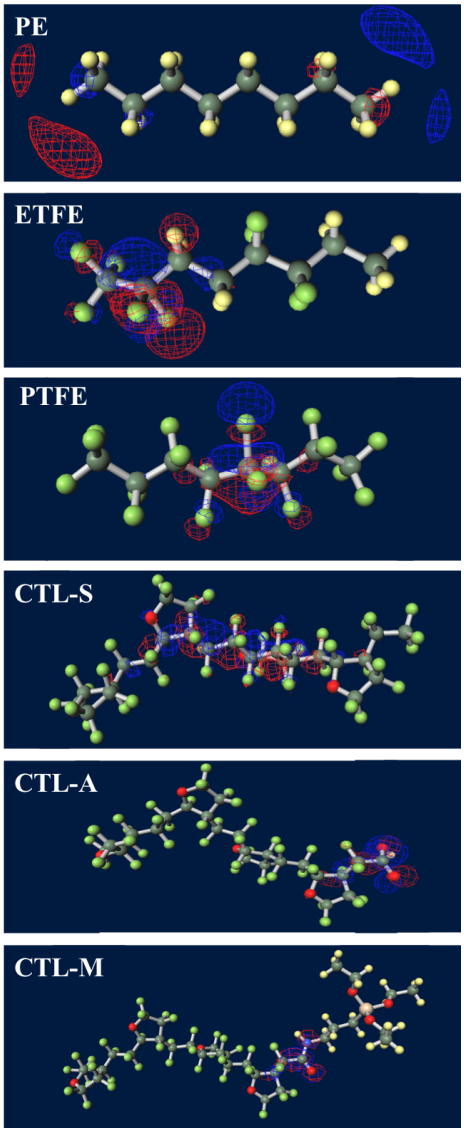

Fig 2. Distribution of trapped electron in electret tetramers (Green: fluorine, Blue: nitrogen, Red: oxygen, Khaki: carbon, Yellow: hydrogen, Pink: silicon)

end group (-COOH of CTL-A and -CONH of CTL-M), implying that the end group attracts the electron even more than perfluorinated back-bone structure itself. The orbital energies of each molecules are calculated. The energy of orbital where the electron is trapped is used to estimate the electron affinity (EA) following Koopmans' theorem. Calculated EAs have order as follows: CTL-M (5.83 eV) > CTL-A (4.7 eV) > CTL-S (4.39 eV) > PTFE (3.56 eV) > ETFE (3.02 eV) > PE (-1.93 eV). Acquired EAs of CYTOP make qualitative agreement with the thermally stimulated discharge (TSD) current peaks [2]. Note that the order of PE, ETFE, PTFE is also in accordance with that of TSD peaks. However, their trap energy cannot be fully described by present simulation because their performance as electret depends on not only by its single molecular EA but also by their morphology. Although our analysis on single molecule cannot perfectly interpret the real system of electret, we expect our method can be used as an indicator to predict performance of amorphous polymer electrets.

The computation is performed with SGI ICE XA ISSP system B F4cpu nodes, using quantum mechanical simulation package NWChem [3]. Every computation was held with 4 nodes (96 CPUs). In case of CYTOP tetramers, the calculation cost was approximately 9200 hours of CPU time for each case. For PE, ETFE and PTFE, 7000 hours of CPU time was necessary in total.

References

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