MERIT internship (domestic) report

Department of Physics
MERIT 9-th
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1 Internship overview

Duration
2022/3/1-2022/3/31
Hosting company
JSR Corporation CURIE

2 Implementation overview

This internship program was conducted both by face-to-face and online at the JSR CURIE office located in Hongo-Campus of the University of Tokyo. During the internship period, We had time to share prucedures every day for about 1 hour and discussed what should we do next. The internship was conducted approximately in 8 hours daily. We presented interim reports for engineers in the Yokkaichi Plant. The final presentations were held for both CURIE and Yokkaichi plant. Also, We visited Bioscience and informatics R&D center (BiRD) for joining the internal seminar.

3 Research

3.1 Background

5G, 6G technologies which realize fast, large-capacity, and low delay communication typically deal with electrical signals of 1THz or higher frequency. This requires materials for 5G,6G communication to have small dielectric-loss in order to prevent high frequency signals to be attenuated. To this end, the design of material molecules must avoid the introduction of polar groups, and if polar groups are introduced, they must be arranged in opposite directions within the molecule so that they cancel each other. As it takes long time to experimentally measure the dielectric loss of materials, the computer simulation for dielectric loss will accelerate material development. We have tackled the computer simulation for dielectric loss of basic organic molecules.

3.2 Method and result

The dielectric spectrum in THz region contains information on the dynamics of picoseconds to sub-picoseconds in terms of time. Among them, Libration is the type of swing motion in which an molecule with a nearly fixed orientation repeatedly rotates slightly. The dielectric loss due to Libration has been measured in many liquids. For example the spectrum of water has the peak oriented from libration at arount 500cm^{-1}. Although benzene is assumed to have low dielectric loss because it has no permanent dipole moment, it actually has the loss due to libration. We calculated the dielectric loss of benzene by Molecular Dynamics (MD) simulation. We confirmed the good agreement with our calculation and the experimental data, and extended this method to molecules with permanent dipole moment. Having discussion with engineers in Yokkaichi Plant, we simulated the dielectric loss of several molecules.

3.3 Impression

I have worked the MD simulation for dielectric loss. Since I have never experienced quantum chemistry, I struggled to understand the calculation result at the begining of the internship, but kind suggestions by staff led me to acquire knowledge of quantum chemistry. Several discussion with engineers in Yokkaichi Plant allowed me to receive valuable opinions from the people working on development, which I believe to make the internshop a fulfilling experience. Also, we visited BiRD, a new research institute, taking infection control measures into consideration, and I was able to actually see a company. It was a good opportunity for me to experience the R&D scene in the industry.

4 Acknowledgement

I would like to express my gratitude to JSR corporation for accepting me for this internship. I would also like to deeply appreciate Itti Rittaporn-sama, Tamio Yamazaki-sama and all the other members of CURIE, for their kind support on this research. In addition, I would like to thank the people from the Yokkaichi Plant for their inspiring discussion. I gratefully thank my supervisor, Professor Shinji Tsuneyuki, who kindly agreed to conduct this internship, and my MERIT associate supervisor, Professor Ryotaro Arita, who approved this internship. Finally, I would like to thank the MERIT program for providing this wonderful opportunity.