Usage Report for Fiscal Year 2016

Project Title:

Intermolecular Interactions in Material Science by Molecular Spectroscopy and First Principles

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Description of the project

1. Background and purpose of the project, relationship of the project with other projects

In this project we aim for investigating the intermolecular interactions by terahertz absorption spectroscopy and quantum chemical calculations. In particular, we are interested in water-polymer interaction, the change of structure and physical properties of polymer materials treated by humidity, observed by THz absorption spectroscopy. The focus of our project is on micro- and macroscopic molecular structure changes (intermolecular interactions and strain degradation) with changing relative humidity. The properties of polymer films change when treated by water vapor, and this phenomenon is of great interest for industry (glass transition temperature, density and several other physicochemical properties).

2. Specific usage status of the system and calculation method

Our original calculations were mostly carried out on GWMPC cluster and in Gaussian 09 quantum chemical software. Anharmonic VPT2 method has been employed on a DFT level for calculation of vibrational frequencies and intensities. Single-hybrid and double-hybrid DFT functionals (i.e. B3LYP/B2PLYP) were mainly used with an appropriate basis set. Where necessary, other levels of electronic theory were employed (MP2, CCSD(T)).

In the FY2017 the project was kept on hold, since the project representative has been involved in other research activity. For this reason, only very limited calculations were performed, mainly aimed at evaluating the potential of BWMPC cluster and Gaussian 16 software (which both became available during FY2017) in theoretical studied of polymer properties.

With the introduction of BWMPC cluster, we plan to move the project to usage of Gaussian 16, as it offers much faster calculation time. We have run BWMPC cluster basing on Intel CPU architecture works much better with Gaussian code, giving substantially BWMPC cluster also is much more potent from the point of view of raw computing power.

3. Result

During FY2017 we have tested the capability of the new BWMPC cluster and Gaussian16 software in computations of polymer properties. We have found out that the combined performance of the new software/hardware gives a substantially lower computational time overall.

4. Conclusion

BWMP cluster and Gaussian 16 software combination gives effectively much better computing times, and the advantage was even higher for frequency calculations of large molecular systems. This enables more adequate studies of polymer fragments.

5. Schedule and prospect for the future

Our plan for the next fiscal year is to continue the computational study of polymer properties within the scope of the project outline.