# Frequency dependent molecular polarizability at near-resonance region using multi-resolution multi-wavelet basis set

Yukina Yokoi*†[1], Tetsuya Kato , Hideo Sekino[1], Robert J. Harrison[2,3], and Alvaro Vazquez-Mayagoitia[4]

[1]Toyohashi Universiy of Technology – Aichi 441-8580, Japon
[2]Institute for Advanced Computational Science, Stony Brook University – Stony Brook, New York 11794, États-Unis
[3]Computational Science Center, Brookhaven National Laboratory – Upton, New York 11973-5000, États-Unis
[4]Argonne Leadership Computing Facility, Argonne National Laboratory – Illinois 60439, États-Unis

**Résumé**

We evaluate frequency dependent (dynamic) molecular polarizability at near-resonance region using multiresolution multiwavelet(MRMW) basis set.
Linear Combination of Atomic Orbitals (LCAO) method have been widely used as an efficient method with a representation of the wave function in general. It has also been used in polarizability calculation. In many cases, Gaussian basis sets have been used.

This method can compute physical property efficiently using less number of basis functions. But if the basis sets is enlarged in order to perform high-precision calculations, computational cost increases exponentially. Because Gaussian basis is designed intuitively, the precision of the calculation cannot be controlled by simply expanding the size of the base functions. Therefore, it is difficult to generate the appropriate space using the Gaussian basis, for molecules that require large freedom of the quantum particle. In order to overcome the problem, we use MRMW basis sets.
MRMW base provides the property computed on the space that approximates the complete space with arbitrary precision, and therefore, the accuracy is ensured automatically, (it can provide a representation space efficiently). We developed a program to calculate the dynamic molecular polarizability with the MRMW basis sets, and the results are compared with the values of polarizability using Gaussian basis sets.

**Mots-Clés:** MRMW, polarizability, basis set

*Intervenant
†Auteur correspondant: yokoi@csc.cs.tut.ac.jp