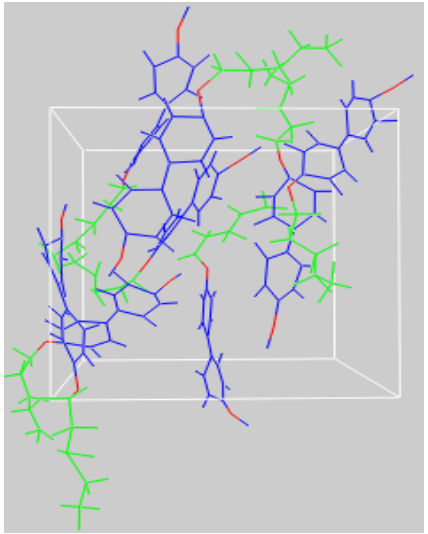
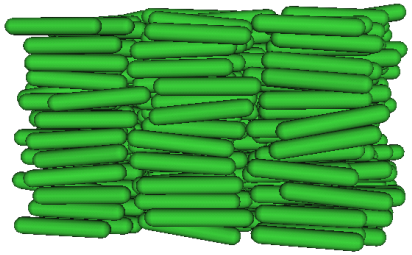
Exploring Materials by Molecular Simulation

Associate Professor Tomonori Koda

I design simulations of atomistic molecules and coarse-grained molecules.



Atomistic model expresses detailed structure of molecules consisting of atoms.



Coarse-grained model extracts specific character of molecles.

Materials are made of molecules. This is a basic stand point of my research for science and engineering. Everything is tried to connect to motion and structure of molecules in my brain. What types of molecules are important for development of novel liquid crystal materials ? How can we express starch molecules in the process of cooking of rice, and what is thermal conductivity in a language of molecules ? These are examples of my curious problems in the world.

In order to discover keys for these problems, I utilize computer to perform molecular simulation. I use atomistic model to describe detail of molecules. I also use coarse-grained models that extract specific features of molecules.

I would appreciate, if you would contact me to consider models for molecular simulations of your interested system. I am happy, when results of my simulation stimulate ignitions of new idea and new technology.

Yamagata University Graduate School of Science and Engineering
Research Interest : Molecular Simulation,
Statistical Physics

E-mail : koda@yz.yamagata-u.ac.jp
TEL（TEL&FAX）: 0238-26-3066