Computational Chemistry at UBE Industries - Tools Used in Cutting-Edge Nanotechnology Applications

Modeling and Simulation Tools Used In New Materials R&D

The R&D department of UBE Industries Ltd. designs new 'specialty chemicals' that deliver high value through inclusion in pharmaceutical products or creating materials with specific functional properties. The manipulation of materials to create functional properties is an important goal of the emerging area of nanotechnology. This technology that controls material structures on the atomistic or molecular level enables the development of unique innovative functions as well as incremental improvements to existing materials and processes. Computational chemistry is exploited by UBE Industries Ltd. as a dominant approach to creating novel nanomaterials.

Modeling and simulation can be used to study material structures at the atomistic and molecular level, allowing existing materials to be refined and new materials designed, often with unique properties. These tools are particularly well suited to the study of nanomaterials.

In looking back almost 15 years, Dr Shigeru Yao, who doubles as Manager of the Materials Design Department and Group Leader of the Nanotechnology Promotion Group in the Polymer Research Laboratory of UBE Industries, reflects on the circumstances leading to adoption of computational chemistry. "Around 1990, while there was a trend towards new polymeric materials development, it appeared that property-estimation methods based on empirical rules had reached their limit. At that point we adopted software that deals with molecular mechanics and molecular dynamics. This was our entry point into the use of computational chemistry."

UBE Industries now uses Accelrys' modeling and simulation tools. Accelrys is a leading supplier of research-support software for life and materials science. UBE uses Materials Studio®, a modeling, simulation, and informatics environment for the chemicals and materials industries. The Materials Studio tools that UBE uses include Discover that calculates molecular mechanics and molecular dynamics, and MesoDyn that calculates coarse-grained dynamics. UBE uses these tools to design materials ranging from polymers to catalysts.

Industry Sectors

Catalysts

Coatings and Additives

Fine Chemicals

Specialty Chemicals

Home and Personal Care

Nanomaterials/Nanoparticles

Organization

Dr Shigeru Yao

Manager of the Materials Design Department

Group Leader of the Nanotechnology Promotion Group

Polymer Research Laboratory

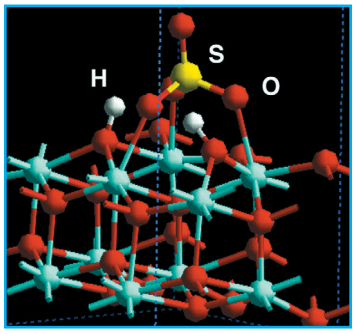
Corporate Research & Development

UBE Industries Ltd.

www3.ube-ind.co.jp/en/index.php3

▲ *Shigeru Yao, Manager of the Materials Design Department and Group Leader of the Nanotechnology Promotion Group in the Polymer Research Laboratory of UBE Industries*

Dr Yao continued, "It is now a common occurrence in our organization to hear questions about the results from a simulation. It appears that computational chemistry techniques are becoming more widely appreciated, and routinely used, as the number of our scientists and engineers using Accelrys solutions increase."



▲ *An example of H_2SO_4 dissociative adsorption analysis on the tetragonal(101) face of ZrO_2*

Material Informatics and Future New Materials Development

It is said that the main value of modeling and simulation is the saving of resources, i.e. time and cost, by rationalization of the R&D process.

Dr Yao explains, "You cannot tell whether or not a target function and property are actually obtained until the material is finally made. But this costs both time and money to do. If it becomes clear that the targeted function does not emerge during simulation, you can stop it in the early stages. And, it is very important that the reason can be rationally explained, not simply feeling that it may fail."

Dr Yao continued, "If the R&D process depends on only conventional experiments or the intuitions of the researchers, it is difficult to recommend both 'non-starters' or 'starters,' and then persuade the company to proceed based on this information."

"Especially for young researchers, simulation is a good training for acquiring theoretical thinking. It leads to an understanding of the fundamentals of the phenomena and provides young researchers a basis for asserting their idea to experienced researchers. If experience and knowledge are captured and preserved in a database format, it should at some point become possible for even inexperienced researchers to explore and investigate the potential in new materials. "

By computerizing 'experiences' and utilizing them systematically, the shift towards materials informatics development that helps researchers' target material designs should continue, and the research field of 'materials design' should come into being, Dr Yao insists.