Computational Materials Science for Everyone

Seungchul Kim, Sang-Soo Han, Minho Lee and Kwang-Ryeol Lee
Computational Science Research Center, KIST (krlee@kist.re.kr)

Computational materials science is a rising field within the materials research community. Indeed, the latest conferences, as recent as the 2015 Materials Research Society Fall Meeting, host several symposiums related to computational materials science, including "Big Data Analysis in Materials Science", "Modeling and Theory-driven Design of Soft Materials", "Architected Materials – Synthesis, Characterization, Modeling and Optimal Design", "Advanced Atomic Algorithm in Materials Science", and "Materials Design by Multiscale Computational Materials Science". A key factor behind the growing interest in computational research is the revolutionary progress made in IT technology. With massive amounts of computation now possible at an affordable cost, accumulated knowledge on the materials modeling at the level of electrons, atoms, molecules, and microstructures has enabled the prediction of material structure and property. In conjunction with such technologies advances, public policies such as the Materials Genome Initiative of the United States have significantly promoted the field of computational materials science [1].

Computational materials science opens a new paradigm for materials research, in which conventional limits of experimental research can be overcome. By simulating material behavior for both ideal and extreme conditions, a better understanding of fundamental mechanisms can be attained. An atomic scale manipulation method to control the fine structure of materials can be thus suggested based on this understanding. Furthermore, any novel idea of materials or materials processes can be screened by computer simulation prior to experiment, resulting in saving time and expenditure for the development. This *in-silico* approach was highlighted as one of 10 world changing ideas in 2013 by Scientific American magazine [2]. In contrast, conventional approach in materials science – *edisonian* approach where any novel idea of materials or materials processes are tested via experimentation – is both costly and inefficient in many cases. From this perspective, the "cross-fertilization" of computational materials science and experimental research is an area that must be addressed, its importance underscored in the 2013 Nobel Prize of Chemistry (Fig. 1) [3].

Despite the importance and value of computational materials science, experimental researchers are usually hesitant to incorporate such tactics to their own research. Because the simulation of materials requires a wide range of fundamental knowledge in materials theory, algorithm, computer programming, and the operating system of a super computer, many find it easier to simply find an expert in the field. Unfortunately, it is not always an easy task to find a collaborative computational researcher interested in a specific project.

One way to bridge the gap is through a web-based simulation platform for non-specialists, such as the one provided by the Computational Science Research Center (CSRC) at KIST (http://vfab.org). Developed for specific applications, the basic concept of the platform is to provide a simulation working environment as a virtual lab to closer mimic experimental research workflow

[4]. This platform is thus distinguishable from existing platforms such as *nanoHUB.org* where a graphical user interface is provided for running a specific simulation code. The KIST platform is designed for use with a minimum level of simulation theory and technical know-how. Users do not need to consider any input parameters directly related to the computation, and only need to define the sample, materials process condition, and method of analysis – as they would in an actual laboratory. The platform then performs the simulation using the pre-defined conditions optimized for the specific process or analysis. The simulation conditions used are determined by the computational researchers based on their own experience. Granted that the computational conditions end up being a black-box to platform end-users, they are provided with documentation containing all technical details from which the capacity and limitations of a simulation can be collected. Figure 2 shows screenshots of virtual laboratories currently under development at KIST.

The platform of this concept might be realized since several simulation methods have been developed to the point that calculations can be performed almost automatically. Yet, the advancement of elaborate computational techniques are necessary for an even more robust materials design platform. First of all, the accuracy and speed of quantum mechanical calculations need to be improved. Development of interatomic potentials is essential for the simulation of a wider range of materials. Especially, a database of the interatomic potentials – one that can be seamlessly applied within the simulation code – is necessary. Limit of time scale of materials simulation is also an important prerequisite for more powerful materials simulations. Finally, novel methods to simulate electrochemical or photon-electron interactions are desirable. Such points of improvement will undoubtedly be tackled on by experts in the field of computational materials science, which will further improve the accuracy and usability of virtual labs for the end-user researcher.

Acknowledgement

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References

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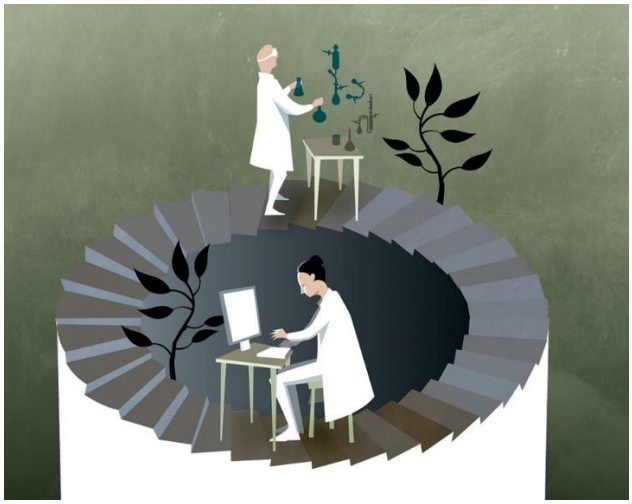

Figure 1. Today, chemists experiment just as much on their computers as they do in their labs. Theoretical results from computers are confirmed by real experiments that yield new clues to how the world of atoms works. [3]

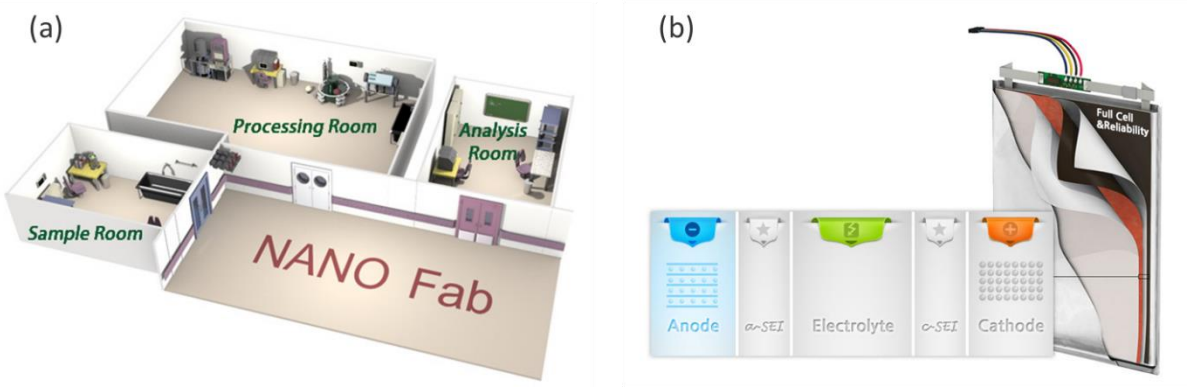

Figure 2 Gates to virtual laboratories. (a) Virtual Nano Fab (http://nano.vfab.org) (b) Battery Materials Design Lab (http://battery.vfab.org)