Computational Materials Science by using the New Supercomputer in IMR - 27 Years with Prof. Kawazoe

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Computational materials science has become more and more important to develop new materials. And also, large computers, especially supercomputers become a powerful tool in materials science. I joined the Prof. Kawazoe's group in 1995 to broaden my research field for materials science.

Our group used first principles calculation and Monte Carlo method mainly to investigate many kinds of materials, in the last two decades. We investigated some novel properties of materials by using Prof. Kawazoe group's program codes. Namely we evaluated some properties that cannot be handled by any commercial code. Complying with this trend, we investigated some properties of actual materials by using various computational methods, so-called multiscale approach. I was particularly interested in novel nanomaterials, energy-related materials, alternative materials for rare metals, and design of advanced materials without hazardous element. To investigate wide range of physical phenomena in these materials, our group has been developed and implemented some program code from hydrodynamics simulation to first principles calculation, including classical MD, Monte Carlo method, and model calculation.

During my employment period in Tohoku University, I was also involved in procurement, management, and tuning of supercomputer in IMR, Tohoku University. In this presentation, I will present some typical and impact results, those are obtained by the supercomputers in IMR.

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References

[1] http://www-lab.imr.edu/~ccms/Eng/