Atomistic Simulation of Materials

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Prediction of structures and properties of materials from the knowledge of their chemical composition has been a longstanding problem in materials science. So far, many inventions with associated improvements have been made to simulate materials structures and properties quantitatively from first principles, *i.e.* starting from the Coulomb interaction between atoms and electrons without using empirical parameters.

The density functional theory (DFT) is one of the most popular bases of the first-principles simulations, for which W. Kohn got the Nobel Prize in chemistry in 1998: with DFT, after some approximations for practical use, we can obtain electron distribution and forces acting on atoms in materials. Sometimes coupled with molecular dynamics method for treating motion of atoms, the theory has been successfully applied to simulations of electronic band structures, crystal structures, surface reconstructions, the structure of liquids or amorphous states, and so on. Nowadays the method is indispensable in various fields of physics and chemistry, and its application to biology is also under way. Theoretical background of the first-principles simulations will be reviewed in the first talk together with very recent progress in the electronic structure theory to go beyond DFT.

As the simulation targets gets larger and more complicated, however, simpleminded application of first-principles simulations easily encounters its limitation due to divergently increasing computational cost. Such examples are found in formation of alloys with microscopic orders, crystal growth and catalytic reactions at surfaces. State-of-the-art applications of DFT combined with different computational schemes in these subjects are also reviewed in successive two talks. Atomistic simulation of protein folding is another example of the highest complexity, where new sampling schemes with unconventional statistics are adopted recently. The new schemes will be reviewed in the last talk.

In conclusion, the purpose of this session is to see how computer simulations contribute to expand the frontier of science.