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Editorial

Preface

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Materials have been playing a role of solid carrier for the advance of human civilization and representing the development level of human productive forces. Human society makes unceasing progress from the Stone Age, Neolithic Age, Bronze Age, Iron Age, to the present information society and times for electronic and various functional materials. All the advances of science and technology rely heavily on the support of materials. Since the industrial revolution in modern times, the development of advanced materials and manufacturing industry has enabled the western countries to maintain a powerful advantage in the global competition. The development and application of new materials reply constantly on the trial-and-error practice by materials scientists, engineers and technicians since the dawn of human society. The reliability of this paradigm of experimental verification and validation is undeniable. However, how to force the slow development of materials to keep up with the rapid pace of industrial product design represents a grand challenge and also an opportunity for materials researchers and producers.

The United States President's Council of Advisors on Science and Technology and the US think-tanks have already realized the hidden troubles in the advanced manufacturing industry. That is, the development of advanced materials has not progressed in a rapid pace as expected and it is difficult to shorten the optimizing period of existing materials. The development of new materials thus becomes a bottleneck in the process of industrial product design. This situation would potentially threaten the pillar industries (such as electronics, automotive and aerospace) that drive the US economy. On June 24, 2011, the White House Office of Science and Technology Policy reported that, the President Obama announced an ambitious plan, the Materials Genome Initiative (MGI), to promote a renaissance of American manufacturing. This initiative is planned to develop a materials innovation infrastructure that consists of computational tools, experimental tools, digital data and collaborative networks, to provide the entrepreneurs and innovators with a wealth of practical information to develop new products and processes, to deepen the understanding about the fundamentals of materials science, and to accelerate the speed of discovery, development, and manufacture of new materials. MGI emphasizes the coordination of computer simulations, experiments and databases, and its contribution to the fast development of new materials.

Currently the materials research level of China falls behind the western countries, and a large number of high-end and high value-added materials have to be imported. The launch of MGI provides us an opportunity to alter the situation of the materials research in China. In recent years the government investments on the research infrastructure at all levels greatly improve our research environment. Advanced internet and convenient literature searching system facilitate the access to up-to-date information and data, ensuring a timely grasp the latest trend in the global materials development. Domestic steel industry has taken the lead in realizing the importance of calculations and simulations. Computer software performing thermodynamic calculations, kinetic simulations and dedicated databases has been introduced to develop high value-added steels. Universities and institutes in China have conducted fundamental researches on first-principles calculations,

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molecular dynamics, materials characterization and property measurement, computational thermodynamics and kinetics, finite element analysis, multi-scale calculations as well as materials databases.

This special issue attempts to review the current situation on materials computations and applications in China, and present several work on the frontier of computational materials science. We should seize the opportunity to convert the paradigm of materials research, construct our own materials innovation infrastructure, and turn materials innovation into a driving force for promoting our manufacturing industry and economy growth.