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Multi-Physics Simulation by Quantum Chemical Molecular Dynamics

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Summary

The establishment of the process and material design technology based on theoretical science at electronic- and atomic-level is one of the important subjects in order to solve the energy and environmental problems, to realize the safe and secure society, and to create new industry and markets. Especially, the recent material, process, and system technologies constitute of multi-physics phenomena including chemical reaction, friction, impact, stress, fluid, photon, electron, heat, electric and magnetic fields etc., and then the deep understanding of the above multi-physics phenomena are essential. Previously, continuum simulations such as finite element method have been employed for the investigation on such complicated multi-physics phenomena. However, quantum chemical approach is essential for the elucidation of the chemical reactions. Then, we recently succeeded in the development of new multi-physics simulator based on our original tight-binding quantum chemical molecular dynamics method, which enables us to simulate the multi-physics phenomena including chemical reactions in addition to friction, impact, stress, fluid, photon, electron, heat, electric fields etc. Moreover, we applied the above simulator to a wide variety of energy problems, environmental problems, and nano-technologies. For example, the realization of super-low friction in"car engine is essential for reducing carbon dioxide emissions and saving energies and resources. Diamond-like carbon (DLC) has received much attention as a super-low friction material and then we investigated the super-low friction mechanism of the DLC via our original multi-physics quantum chemical molecular dynamics simulator. The simulation results suggested that the surface termination of the DLC by hydrogen is essential for the super-low friction. Especially, it is the very interesting that hydrogen molecules generated at the friction interface and the generation of hydrogen molecule leads to the super-low friction. We also applied our multi-physics simulator to the fuel cell, solar cell, semiconductor process, chemical mechanical polishing etc. The detailed information on our successful applications can be seen at http://www.kubo.rift.mech.tohoku.ac.jp/eng/theme.html.