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## Molecular design for automotive tribology

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In order to image the future of social mobility, we need to consider many options. The most traditional one is to consider the combustion engine. There are still needs to increase fuel efficiency, improve the maintenance free system. On the other hand, growing the number of electric vehicles makes new friction control for especially for the high-speed ball bearings. Fuel cell car is still a candidate for the mobility, since hydrogen is the real clean energy resource. In this point, we need to consider hydrogen effect on the many kinds of steel. Since the automotive industry is a huge in the world, the manufacture process should be clean.

To attack these above problem, molecular simulation of tribology is adoptable in many research topics. In this talk, we will introduce an example of analysis of interface science using molecular simulation as a method for automotive tribology. For a hydrogen society, we will introduce analysis of low friction and wear surface coatings and hydrogen storage materials. Regarding PFAS, we explain SDA (hierarchical dipole array) model, which is a physical chemistry theory originating in Japan, to understand the origin of functions such as water and oil repellency and how to understand these kinds of molecular feature. The simulation results support and expand the theory very well. Multiscale, multiphysics is the key concept to model such a system. We built up two simulators, one is the SPH (smoothed particle hydrodynamics) simulator to treat friction and wear in micron scale[1-3]. The other is fluid-molecule hybrid simulator to simulate complex fluids such as lubricants[4-6]. Supercomputers are said to be like telescopes peering into the future. I would like to discuss the prospects of molecular simulation that will encourage the Tribology society by making full use of supercomputers.

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