Tribochemical Reaction Dynamics of Diamond-Like Carbon and Its Related Materials by First-Principles and Tight-Binding Quantum Chemical Molecular Dynamics Simulations

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Diamond-like carbon (DLC) and its related materials have gained much attention as super-low friction materials for automotive engines, aerospace equipments, and so on. The detailed understanding of the tribochemical reactions of the DLC and its related materials is strongly required for clarifying their super-low friction mechanism and designing more efficient super-low friction materials. Here, classical molecular dynamics simulation is frequently employed to investigate the friction behaviors on atomic scale. However, the classical molecular dynamics method cannot simulate the chemical reaction dynamics. Therefore, we developed our original first-principles molecular dynamics simulator "Violet" [1] and tight-binding quantum chemical molecular dynamics simulator "Colors" [2] for the elucidation of the tribochemical reaction dynamics of DLC and its related materials [3,4]. Our successful application to the tribochemical reactions of methanol molecule in DLC was demonstrated in the cover picture of the Faraday Discussions, Vol. 156 (Figure). In this symposium, we will introduce various applications of the first-principles molecular dynamics simulator "Violet" [1] and tight-binding quantum chemical molecular dynamics simulator "Colors" [2] to the tribochemical reaction dynamics of DLC and its related materials.

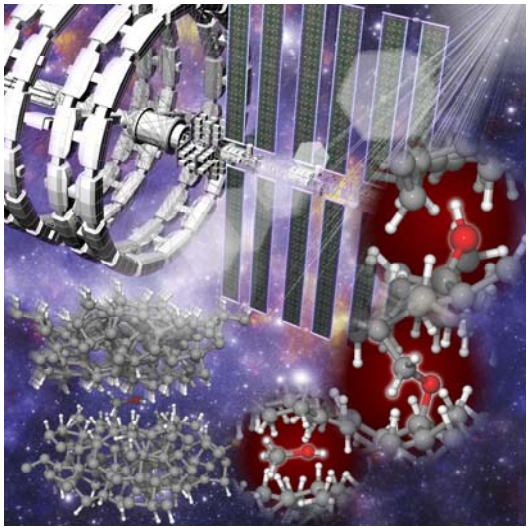

Figure Tribochemical reactions of DLC in aerospace equipments.

[1] T. Shimazaki and M. Kubo, Chem. Phys. Lett., 503 (2011) 316.
[2] M. Koyama, M. Kubo, A. Miyamoto et al., J. Phys. Chem. B, 110 (2006) 17507.
[3] K. Hayashi, M. Kubo et al., J. Phys. Chem. C, 115 (2011) 22981.
[4] K. Hayashi, J.-M. Martin, M. Kubo et al., Faraday Discuss., 156 (2012) 137.