Molecular Dynamics Simulations of Water and Hydrogen Formation on Lunar Surface Z. Huang[1], K. Nomura[2], A. Nakano[2], J. Wang[1](josephjw@usc.edu) [1]Department of Astronautical Engineering, University of Southern California, Los Angeles, CA, 90089. [2] Collaboratory for Advanced Computing and Simulations, Department of Chemical Engineering and Materials Science, Department of Physics and Astronomy, and Department of Computer Science, University of Southern California, Los Angeles, CA, 90089

Introduction: While the existence of water and hydroxide molecules has been confirmed on the Moon by observations and predicted on certain asteroids, the exact process underlying the origin of water is still under debate. It is commonly agreed that solar wind proton implantation is a major source for hydrogen in the hydroxylation process. However, the detailed mechanism underlying the water formation process is not clear. This paper presents two studies on the water formation mechanism. One focuses on the lunar terminator permanently shadowed regions (PSRs) and the other focuses on the low longitude day-side region. Both studies are based on molecular dynamics (MD) simulations.

Simulation Model: The simulation model used is a reactive molecular dynamics simulation model, RXMD, recently developed at USC. Reactive molecular dynamics is a computational materials modeling method that follows the time evolution of the positions of each atoms in material by numerically integrating Newton's equations of motion. In the simulation, the atomic energy and force used are derived from the reactive interatomic force field, a first-principle informed reactive force field that describes chemical reactions. Compared to quantum mechanics based methods, RXMD significantly reduces the computational cost while retaining the description of the energy landscape obtained from quantum-mechanics calculations.

Water Formation in the PSRs: In the lunar PSRs, the surface temperature is too low for most candidate reactions related to water formation to occur. We propose that the electric field from space weather induced dielectric charging in lunar regolith is the catalyst for water formation in the PSRs. To investigate this hypothesis, we consider a lunar regolith grain surrounded by solar wind implemented hydrogens in a surface with a temperature of 40K. The regolith grain is modeled as a hydroxylated silica nanoparticle. The electric field from deep dielectric charging is taken to be 5×10^6V/m. Under the applied electric field, the crystal silica structure in the regolith is broken along with the hydroxyl groups on the surface, and the oxygen is desorbed. At the end of the simulation, a significant amount of water molecules are formed, and are attached to the silica surface (Figure 1). While the exact amount of water formed depends on many factors, such as the strength of the electric field, the surface temperature, the density of the implemented hydrogen in the lunar soil, and the size of the regolith grains, about 15% of the oxygen atoms in the SiO_2 nanoparticle react with hydrogen to from water in the simulation setups considered.

Water/Hydrogen Formation in the Low Longitude Day-side Region: In the low longitude, day-side region, we find that the lunar surface temperature and the energy from solar wind impingement on the surface are sufficiently high to induce water and hydrogen formation. MD simulations are carried out to study solar wind impingement on a regolith surface with a temperature of 300K. Different solar wind speeds are used to represents the impingement at different longitudes and the space weathering effects. The results show that a considerable amount of hydronium ions are formed at lunar lower longitude surface. As these ions are evaporated from the surface (Figure 2), lunar surface charging will play role in the transport and distribution of water on lunar surface.

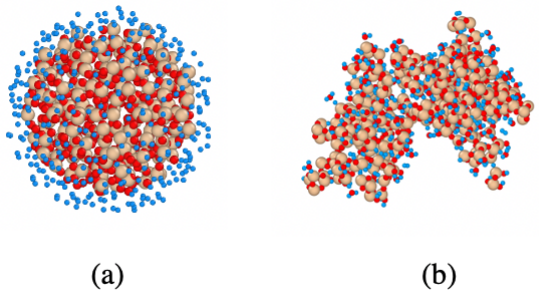

Figure 1: Simulation of Water Formation induced by Electric Field. Yellow particles represent silicon atoms, red particles represent oxygen atoms and blue particles represent hydrogen atoms. (a) is the setup configuration, (b) is the structure after a SEP event.

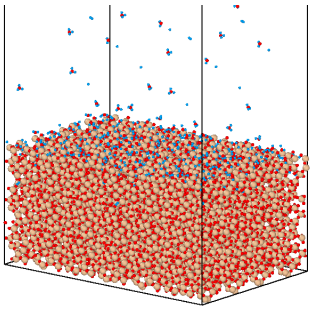

Figure 2 Solar Wind Impingement Simulation. Same particle configuration in Figure 1. H_3O^+ are evaporated from the surface.