On the Importance of Determining Binding Energies of Volatiles on the Moon

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Despite the label as an "airless body", volatiles exist on the Moon. Such volatiles were either delivered, present at the lunar formation event or made *in situ*. Understanding the detailed interactions of water and other volatiles on the Moon is an extremely complex problem and, as documented below, is a major priority in science and human exploration of the Solar System. Knowledge of how water and other volatiles interact with lunar regolith is necessary to constrain the origin of such volatiles, and to understand current and future mission data sets. Furthermore, understanding lunar volatile migration and transport are critical for selection of potential ISRU sites and can support pre-mission planning.

Impacts deliver water and other volatiles to the Moon [1, 2], while the synthesis of chemically bound hydroxyls in lunar regolith grains is attributed to solar wind implantation [3-5]. In addition a small amount can also be formed diurnally [6]. The heated lunar surface and interface reactions of hydrogen enriched regolith (i.e. -OH implanted defects) follow a well-known pathway described by the mechanism of recombinative or associative desorption. Briefly, recombinative desorption (RD) is a reaction and desorption event that occurs between neighboring hydroxyl defects, $-OH + -OH \rightarrow O + H_2O(g)$. Our previous work demonstrated that a small number (~30%) of the total sites produced by the solar wind on an Apollo mare sample (10084) were available for recombinative desorption during normal dayside temperatures on the Moon [6]. We were able to show that solar wind implantation and subsequent recombinative desorption can explain the latitude dependence observed in the M^3 dataset [7, 8]. Knowledge of volatile binding energies will achieve the following science goals.

Ascertain and constrain the origin of volatiles on the Lunar Surface:

As discussed above, the recombinative desorption mechanism is a potential source term for water on the moon and other airless bodies in the solar system. Although previous research has focused heavily on the formation of water, the mechanism of recombinative desorption is universal and applies to other volatiles originating with defects created through solar wind implantation, e.g. proton and carbon ions resulting in the formation of methane [9, 10]. Temperature program desorption is the ideal method for determining the binding energies of adsorbed volatiles and activation energies of volatile production. From these activation energies and the overall shape of the desorption profile, conclusions can readily be made on the origin of the volatile. For example, if water is physisorbed on the regolith in multilayer concentrations (e.g. ice layers), the desorption profile of water as the soil is heated will be narrow with a sharp drop off and very low activation energy (<50 kJ mol^{-1}). However, if water is chemisorbed at the monolayer or submonolayer concentrations, the desorption profile will be asymmetric with midrange (50 – 100 kJ mol^{-1}) activation energies. Finally, if water does not appear until high temperatures with a very broad distribution profile, this implies recombinative desorption from solar wind created defects. For a given laboratory sample or path of lunar surface, it is likely that all three situations will be observed. However, the profiles can be disentangled from one another. The quantity of water observed for each desorption mechanism can reveal clues to the origin as well. For example, a delivery mechanism (implying large amounts of molecular water) would produce a low temperature water feature in higher quantities than the high temperature water desorption feature. Further, if similar quantities of water were observed in old and young lunar soil, this again would imply a delivery mechanism. Conversely, if more high temperature water was observed in old vs. young soil, this would imply water of a predominantly solar wind origin.

Quantify how volatiles interact with the lunar regolith.

Water is a necessary resource for planned human exploration and habitation on the moon. Knowledge of water binding energies on lunar regolith is crucial to understanding the transport of water on the lunar surface. Ultimately, quantification of volatile binding energies and abundance of binding sites will allow for the prediction of where and how much and where on the lunar surface water can accumulate and the potential that it can be extracted for human use. Not only does precise measurement of the binding energies allow for prediction of potentially important sites for ISRU, it allows for the understanding of what governed the accretion of water and how space weathering affects potential binding sites. While the local temperature plays a significant role in the lifetime of a physisorbed or chemisorbed volatiles, the activation energy is the controlling parameter. Furthermore, exposure to the atmosphere can "heal" defects created by solar wind sputtering by dissociatively adsorbing at these defect sites, thereby altering the distribution of binding energies. Laboratory based measurements on recovered Apollo samples will inevitably share this problem, highlighting the need for more advanced *in situ* measurements.

Quantify the depth profiles and total amount of volatiles residing in the lunar regolith.
Volatiles within the lunar regolith are of immense importance due to their potential for supporting human exploration. Depth concentration profiles arise from the simple fact that volatiles trapped deeper within the porous regolith will arrive later that those nearer the surface. The time evolution will depend heavily on the porosity of the regolith and the local pressure as this dictates the collision frequency of the gas phase volatiles [11]. In addition, binding energies of the regolith will significantly affect the desorption profile as re-adsorption will occur as well [12]. Consequently, resolving depth concentration profiles can reveal detailed information necessary to understand gas transport as well.

Predict areas of high volatile concentrations and provide high level data for mission planning.
Simply put, long term human habitation and exploration of the lunar surface will be severely hindered, or even economically impossible without the *in situ* extraction and utilization of resources. Generally, the PSRs of the moon are thought to be the area with the highest concentration of volatiles as these areas act as geologically stable cold traps. However, the lack of sunlight and cold temperatures present a severe engineering challenge, not to mention the danger posed to a human astronaut. Without the sun to recharge the battery packs or long, heavy tethers, any mining equipment will be limited in duration with even less time as energy is wasted traversing in and out of the crater. Binding energies will provide data that can inform planning to assure that goals for exploration missions are met. Furthermore, prediction of volatile migration and transport allows the forecasting of potential ISRU sites with an increased confidence thereby supporting mission planning of Artemis human exploration missions

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