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A Combined Computational and Experimental Approach to Investigating Volatile-Surface Interactions on Airless Planetary Bodies

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Introduction: The surfaces of airless, planetary bodies like the Moon and Mercury are constantly exposed to several processes that eject atoms into the exosphere[1,2]. While the composition and densities of these exospheres are partially known based on observational data from exploratory missions[3], the source of each component is not well understood. This uncertainty necessitates better constraints for accurately interpreting the observed exospheric data, which requires both experimentally constrained measurement and atomistic-level physical insight.

Laboratory studies provide valuable measurements of adsorption and desorption behavior, while molecular dynamics (MD) simulations enable direct investigation of the atomic-scale interactions that cannot be resolved experimentally. By combining these approaches, it becomes possible to better constrain the physical mechanisms controlling surface-exosphere interactions on bodies such as Mercury and the Moon.

In this work, MD simulations of Na and K adsorption on silica surfaces are combined with thermal stimulated desorption (TSD) experiments of Na and K adsorbed onto silica. The study focuses on understanding how surface coverage and environmental hydroxylation influence adsorption energetics and desorption behavior[4]. The combined computational and experimental approach not only provides validation between methods, but also demonstrates how MD simulations can explain experimentally observed trends and identify surface processes relevant to planetary environments.

Methodology: MD simulations were performed to investigate Na and K adsorption on silica surfaces under varying surface coverages and surface chemistries. Surface binding energies (SBEs) were calculated for adsorbed Na and K atoms to quantify the strength of adsorbate-surface interactions and to identify how adsorption behavior evolves from isolated adsorbates to high-coverage surfaces[5]. Additional simulations examined H covered silica surfaces to evaluate the effect of hydroxylation on adsorbed Na SBEs.

TSD experiments were conducted by collaborators using Na- and K-dosed Apollo samples[6]. Following adsorbate deposition, samples were heated to approximately 1000K while monitoring desorption behavior to derive activation energies associated with adsorbate release from the surface. The experimental desorption energetics were compared directly with the MD-derived SBEs to investigate

the physical origins of the experimentally observed desorption behavior.

Results: The combined MD and experimental results demonstrate strong agreement between stimulated adsorption energetics and experimentally observed desorption behavior. Figure 1 displays the SBE distributions of adsorbed Na on a bare silica surface, Na covered surface, and hydroxylated surface.

MD simulations show that isolated Na atoms adsorbed directly onto bare silica surfaces form strongly bound adsorption states with SBEs exceeding 5 eV. These energies are larger than the effective experimental detection range of the TSD studies, which are insensitive to adsorption energies above approximately 3.5 eV at the maximum experimental temperature of 1000K. Consequently, strongly bound adsorbates detected in the MD results are unlikely to desorb during experimental heating cycles.

This provides important insight into the physical experiments, suggesting that residual adsorbates likely remain on the silica surface between experimental runs despite minimal dosing conditions. Over time, this accumulated coverage may produce increasingly significant Na-Na or K-K interactions and lower-energy adsorption states, consistent with the experimentally observed desorption energies. In this way, the MD simulations provide a physical explanation for experimental behavior that cannot be directly measured.

Further MD simulations demonstrate that hydroxylated silica surface significantly reduce adsorbate SBEs relative to bare silica (by ~2.9 eV). This suggests that exposure of experimental samples to ambient atmospheric water or H during sample transfer may hydroxylate undercoordinated surface oxygens, producing weaker adsorption states and lower desorption temperatures in the TSD measurements. Similar hydroxylation processes are also expected on Mercury and the Moon due to solar wind hydrogen implantation, likely resulting in spatially variable adsorption energetics across the planetary surface.

Together, these results demonstrate how combining MD simulations with laboratory experiments enables a more reliable interpretation of both datasets while providing improved insight into the surface processes governing volatile behavior on airless planetary bodies.

Conclusion: This study demonstrates the strength of integrating MD simulations with laboratory thermal desorption experiments to investigate surface processes on airless planetary bodies. While experiments provide direct measurements of adsorbate desorption behavior, MD simulations reveal the underlying atomic-scale interactions responsible for the observed trends. The combined approach identifies the important roles of surface coverage and hydroxylation in controlling adsorption energetics and explains how experimentally inaccessible strongly bound adsorption states may influence measured desorption behavior.

By coupling computational and experimental methods, this work provides a more physically complete understanding of adsorbate-surface interactions and highlights the importance of considering realistic surface environments when interpreting laboratory measurements and modelling planetary surface-exosphere systems.

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