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# Uncovering the Role of Hydroxylation and Oxygen Depletion on the Surface Binding Energy of Adsorbates: A Molecular Dynamics Study

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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 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. While complex laboratory studies drive reliance on theoretical models to study these exosphere-surface interactions.

Molecular dynamics (MD) simulations rely on interatomic potentials to model interactions at the atomic level without requiring user-provided inputs. However, their high computational load restricts the size and timescale of simulations. As an alternative, MD can be employed to determine critical mineral-specific parameters, such as the surface binding energy (SBE), that can then serve as inputs for large-scale ejection models.

This methodology has been used to study mineral-specific SBEs of both crystalline and amorphous surfaces[4,5]. More recently, we also considered the effect of adsorbates (i.e., atoms that eject below the escape energy and return to the surface) on SBE and subsequent emission processes for crystalline and amorphous surfaces[6]. However, the surfaces of these planetary bodies are much more complex than has been considered in these studies. For example, space weathering causes transient or localized hydroxylation of surface minerals via solar wind proton interactions[7], as well as dynamic oxygen depletion due to preferential sputtering[8]. No study has considered how these different structures will affect the SBE and subsequent predicted exospheres. Without considering these complexities the MD derived SBEs are limited in their application to exosphere modelers.

**Methodology:** This study evaluates the adsorption of Na onto hydroxylated and oxygen depleted $SiO_2$, albite, and anorthite, determining SBE distributions using MD simulations.

**Results:** Figure 1 displays the SBE distributions of adsorbed Na on 100% hydroxylated and clean (i.e., non-hydroxylated) $SiO_2$, albite, and anorthite surfaces.

Figure 1. SBE distributions of adsorbed Na on the hydroxylated surfaces of $SiO_2$, albite, and anorthite. The whole lines represent the hydroxylated SBE distributions of each surface, and the dashed lines represent the clean surface (i.e., non-hydroxylated) SBE distributions.

First, it is evident that the hydroxylation of $SiO_2$, albite, and anorthite surfaces results in a distinct shift of SBE distributions and significantly reduces the average SBEs of adsorbed Na. The average SBE of Na adsorbed onto a clean $SiO_2$ surface is 5.7 eV, while the average SBE of Na adsorbed onto a hydroxylated $SiO_2$ surface is 2.8 eV. We attribute these findings to the unique bond types and interactions formed in each case.

In the clean surface models, it is expected that adsorbed Na atoms form ionic bonds with the surface oxygen atoms which have a high bond strength. In the hydroxylated surface models, the surface oxygen atoms are already bonded to hydrogen, reducing its availability for interactions with the adsorbed Na. Instead, Na may be interacting via hydrogen bonding or weak van der Waals interactions with -OH groups, resulting in lower SBEs. These findings align with previous relevant literature[9,10], however future experimental work is required for validation.

In summary, the localized hydroxylation of surface minerals on the Moon and Mercury suggests that lower energy sites are available for adsorbates, making ejection processes of these atoms significantly more efficient. It is therefore paramount to understand the extent of localized hydroxylation on the surface of airless bodies in order to then quantify the contributions of different sources into the exosphere. Next, surface oxygen depletion of these surfaces will be investigated. The development of a database of SBEs that capture the complexities of surfaces on airless planetary bodies is crucial for connecting source processes to atomic species and achieving a complete understanding of the surface-exosphere connection.

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