

**THE EFFECT OF DIFFUSION ON THE BINDING ENERGY OF ADSORBED SODIUM ON THE SURFACE OF MERCURY.** A. Georgiou<sup>1</sup>, A. Ricketts<sup>1</sup>, S. Verkercke<sup>2</sup>, J. McLain<sup>3</sup>, F. Leblanc<sup>4</sup>, M. Sarantos<sup>3</sup>, L. S. Morrissey<sup>1</sup>, <sup>1</sup> Faculty of Engineering and Applied Science, Memorial University of Newfoundland, St. John's, NL A1C 5S7 Canada, <sup>2</sup> LATMOS/CNRS, Université Versailles Saint Quentin, Guyancourt, France, <sup>3</sup> NASA Goddard Space Flight Center, Greenbelt, MD 20771, USA, <sup>4</sup> LATMOS/CNRS, Sorbonne Université, Paris, 75252, France.

**Introduction:** The collision-less atmosphere of the Moon and Mercury allows for several space weathering processes, such as micrometeoroid impact vaporization and solar wind ion sputtering, to take place simultaneously on its surface. Many of these processes can lead to the emission of surface atoms into the exosphere. Observations of atoms in the exospheres of airless bodies are widely considered to originate from these space weathering events [1-4]. Other processes, such as photon-stimulated desorption (PSD), electron-stimulated desorption (ESD), and thermal desorption, are also likely important mechanisms that could eject atoms to the exosphere [5].

Of the several atomic species discovered, sodium (Na) remains the most studied and abundant in Mercury's exosphere. Several different space weathering processes are thought to be potentially important for its ejection into the exosphere. However, the exact contribution of each remains unknown [6-12]. In addition, those atoms ejected with an energy below the escape energy can return to the surface and adsorb at binding energies lower than when bound within the mineral [13]. Due to their lower binding energy, these can be more efficiently re-ejected through PSD, ESD and thermal desorption, which require lower energy than micrometeoroid impacts and solar wind sputtering.

It is unknown whether the diffusion of adsorbates along the surface can dynamically affect the binding energies by changing its value, affecting the ejection of the adsorbed atoms. Here, we use molecular dynamics (MD) modelling to study the dynamic behaviour of Na adsorbates on the surfaces of key silicates and feldspars relevant to the Moon and Mercury. Our simulations consider the atomic mechanism of adsorption, allowing the adsorbates to diffuse and eventually desorb with time. We investigate how the distribution of binding energies changes with temperature, time, crystallinity, and surface composition.

**Methodology:** We performed MD simulations using a reactive (ReaxFF) potential on the two endmembers of the plagioclase feldspar group, albite (NaAlSi<sub>3</sub>O<sub>8</sub>) and anorthite (CaAl<sub>2</sub>Si<sub>2</sub>O<sub>8</sub>), which are thought to be abundant on the surface of the Moon and Mercury. We also considered silica (SiO<sub>2</sub>), which is found on Mercury's surface at 49 - 55 wt.%. Our simulations included both crystalline and amorphous structures. After the preparation of each slab, ~240 Na atoms

were randomly placed at 5 Å above the surface and allowed to adsorb on the surface at 100 K, 300 K and 700 K with the adsorption energy recorder after 100 ps of simulation time. After the initial adsorption energy at time 0, each system was then kept at the desired temperature for an additional 4000 ps. We calculated the Na atoms' MSD and binding energy during the simulation run and tracked the surface desorption.

**Results:** Results clearly indicate how the surface composition can influence the initial sampled adsorption energy. We observed no distinct differences in initial adsorption energy with changes in temperature and crystal structure. The presence of Al/Ca and Al/Na in anorthite and albite, respectively, reduces the adsorption energy of the Na on the silicate, with silica exhibiting the highest energy. In addition, the presence of Al/Ca and Al/Na in the substrate also limits the diffusion of adsorbed Na atoms. We found that diffusion of Na atoms is also restricted in crystalline substrates compared to amorphous ones, with Na mobility being higher in amorphous cases. The binding energy has been shown to change with time as diffusion randomly displaces Na atoms to higher binding energy sites on the surface and deeper within the substrate. Furthermore, the desorption of loosely bound atoms can also increase the average binding energy. We also sampled the individual binding energy of the atoms, showing a wide range of binding energy distributions that shifted towards higher values after 4000 ps.

**References:** [1] Broadfoot, A., et al. (1976) *Geophysical Research Letters*, 3(10), pp. 577–580 [2] Cassidy, T., et al. (2016) *Geophysical Research Letters*, 43(21), pp. 11,121–11,128. [3] Quémerais, E., et al. (2023) *Journal of Geophysical Research: Planets*, 128(6), p. e2023JE007743. [4] Vervack, R. J., et al. (2016) *Geophysical Research Letters*, 43(22), pp. 11,545–11,551. [5] Domingue, D., et al. (2014). *Space Sci Rev*, 181, pp. 121–214. [6] Killen, R. M., et al. (2004). *Icarus*, 171(1), pp. 1–19. [7] Leblanc, F. & Johnson, R. E. (2003). *Icarus*, 164(2), pp. 261–281. [8] Madey, T., et al. (1998). *Journal of Geophysical Research: Planets*, 103(E3), pp. 5873–5887. [9] Sarantos, M. & Tsavachidis, S. (2020). *Geophysical Research Letters*, 47(16). [10] Wurz, P., et al. (2010). *Planetary and Space Science*, 58(12), pp. 1599–1616. [11] Yakshinskiy, B., et al. (2000), pp. 75–87. [12] Yakshinskiy, B. & Madey, T. (2003). *Surface Science*, 528(1–3), pp. 54–59. [13] Morrissey, L. S., et al. (2025). *The Astrophysical Journal*, 981(1), p. 73.