

**Supplementary Material for
Simulated Lunar Surface Hydration Measurements using Multispectral Lidar at 3 μm**

Daniel R. Cremons and Casey I. Honniball

This file contains the following sections:

- Comparison of the 3 μm Feature from Remote Sensing, MORB Glass, and Synthetic Spectra
- Removal of Terrestrial Organic and Water Features from Endmember Apollo Spectra
- Normalization and Interpolation Methods for Mid-Ocean Ridge Basalt (MORB) Glass Spectra
- Synthetic Lunar Glass Spectra
- Band Depth Effects due to Pyroxene
- Converting Total Water Abundance Error to Band Depth Error
- Multispectral Lidar Signal to Noise Ratio (SNR) Calculation
- References

Comparison of the 3 μm Feature from Remote Sensing, MORB Glass, and Synthetic Spectra

To create spectral mixtures with a known total water abundance, we required sample data for which reflectance spectra in the near infrared and mid infrared were available and for which the total water abundance was determined in a method independent of the 3 μm band. The Mid-Ocean Ridge Basalt (MORB) glass samples have been used to generate a 3 μm band depth vs. total water abundance relationship, and they are a close analog to lunar glasses where significant water abundance may reside. Below are comparisons of MORB glass spectra to remote sensing datasets to highlight the similar band shape and position. Figure S1 shows comparisons of ground-based InfraRed Telescope Facility (IRTF) data from Honniball et al. (Honniball et al., 2020) with scaled MORB spectra overlain. Figure S2 shows orbital spectroscopic data from the M³ spectrometer taken from McCord et al. (McCord et al., 2011) and the EPOXI spectrometer (Sunshine et al., 2009) with one of our simulated spectral mixtures overlain. In both cases the band minima match up well. This example figure also demonstrates our spectral mixtures approximate real remote sensing spectra well.

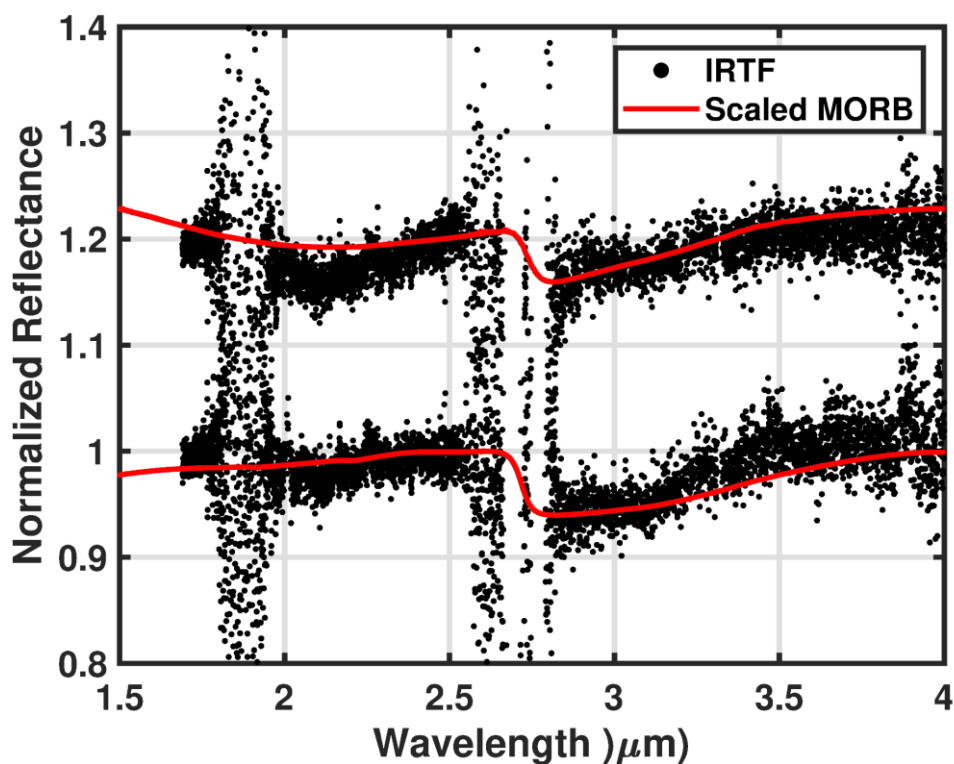


Figure S1. Comparison of remote sensing data from the Infrared Telescope Facility (IRTF) and hydrated MORB spectra. IRTF spectra are from Honniball et al., 2020.

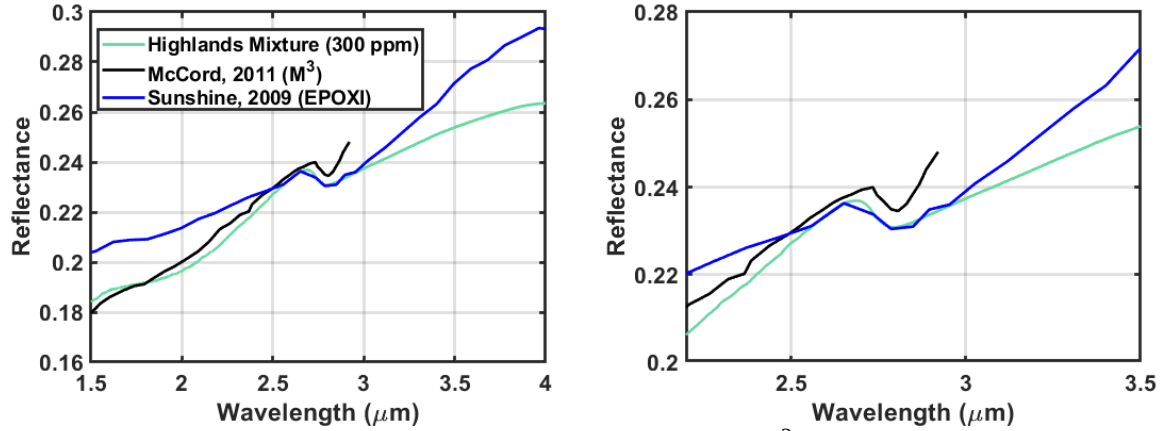


Figure S2. Comparison of lunar remote sensing data from M³ and EPOXI to synthetic spectrum from our simulations.

Removal of Terrestrial Organic and Water Features from Endmember Apollo Spectra

The Apollo soil spectra from the RELAB database all exhibited various absorption features between 2.6 and 4 μm including a characteristic 3 μm water absorption feature and organic doublets near 3.4 μm , indicating the presence of unquantified hydration, likely from a terrestrial source (Figure S3, left). Our goal was to introduce only a known hydration signature to compare with the retrieved value, which meant we must first remove this unknown water signature from the endmember spectra. We performed a linear fit of the reflectance data for the five Apollo samples using anchor points at 2.6 and 4.0 μm , then substituted the linear fit into the component spectrum to remove both the water and organic absorption features. Finally, the component spectra were interpolated to a uniform 5-nm spectral sampling from 1 to 4 μm (Figure S3, right). For reference, the processed mare spectra shown in Figure S3 are comparable to spectra of Apollo 17 mare soils heated to 500 $^{\circ}\text{C}$ under high vacuum by Ichimura and co-authors (Ichimura et al., 2012).

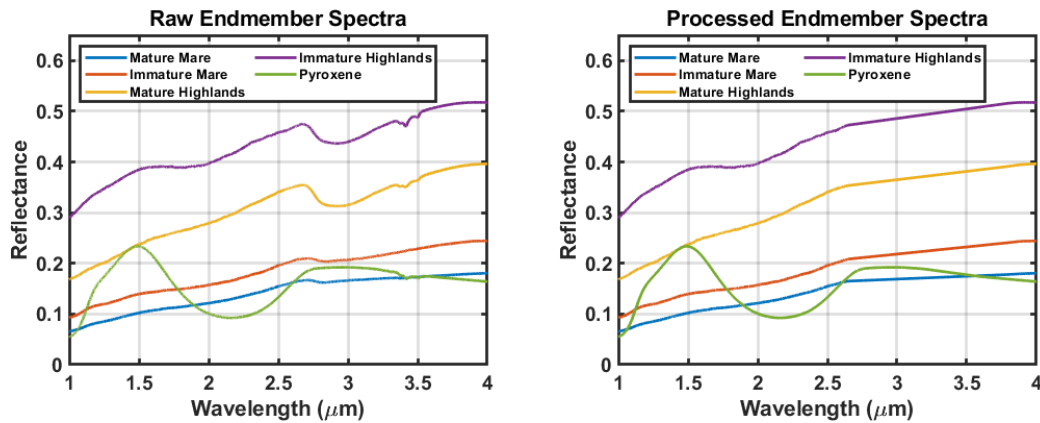


Figure S3. Raw Apollo soil spectra from the RELAB database (left) exhibiting unquantified terrestrial water and organic contamination. Processed spectra (right) with water and organic spectral features removed and interpolated to uniform spectral sampling. Note these spectra are

still for the laboratory viewing geometry of 30/0/30 (incidence angle/emission angle/phase angle).

Normalization and Interpolation Methods for Mid-Ocean Ridge Basalt (MORB) Glass Spectra

Reflectance data from the step-wise heating experiments of MORB D38A were obtained in units of instrument count and required normalization between spectra to isolate the 3 μm band. We normalized the four experimental MORB spectra at a wavelength of 2.6 μm , and appended the low-wavelength region of sample D38A measured separately to cover the entire lidar wavelength range. This process is shown in Figures S4 and S5.

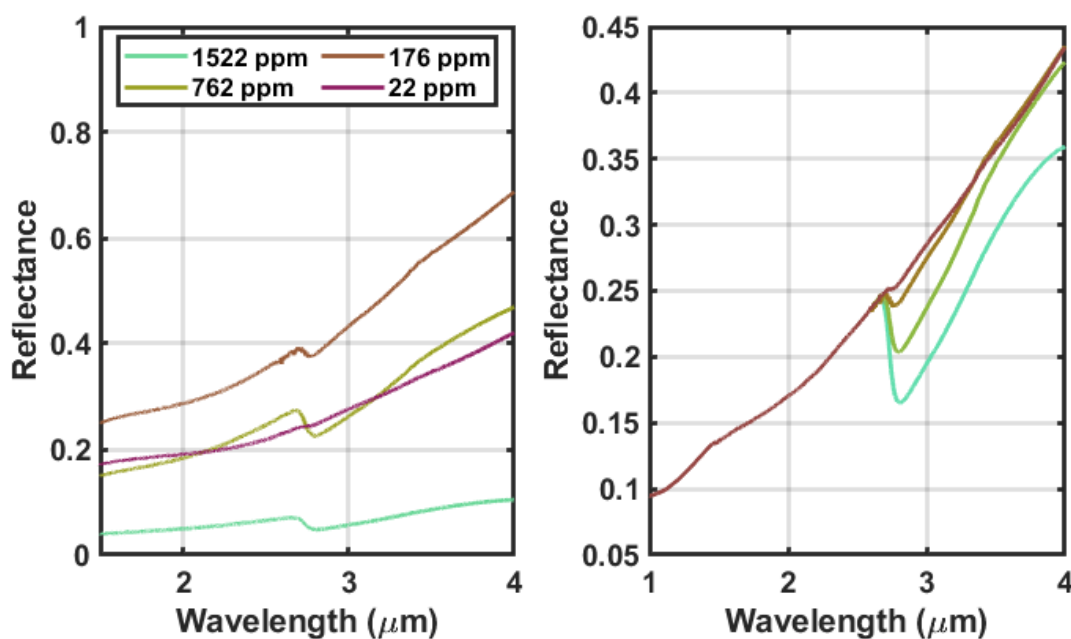


Figure S4. (left) Raw MORB spectra of sample D38A. (right) MORB spectra after normalization at 2.6 μm and appending low-wavelength data.

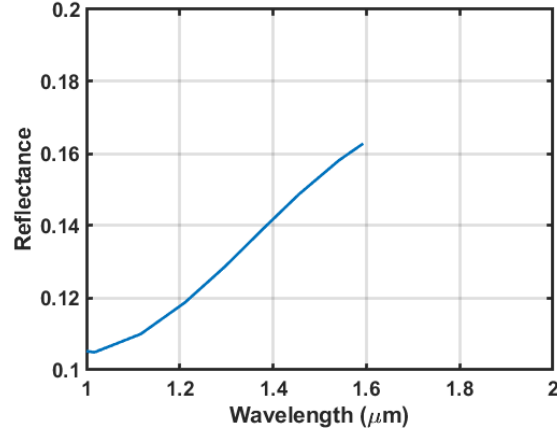


Figure S5. Low-wavelength spectrum of MORB glass sample D38A

We then converted the laboratory reflectance spectra to single scattering albedo using the Hapke radiative transfer model described in the main text. The SSA spectra are shown in Figure S6.

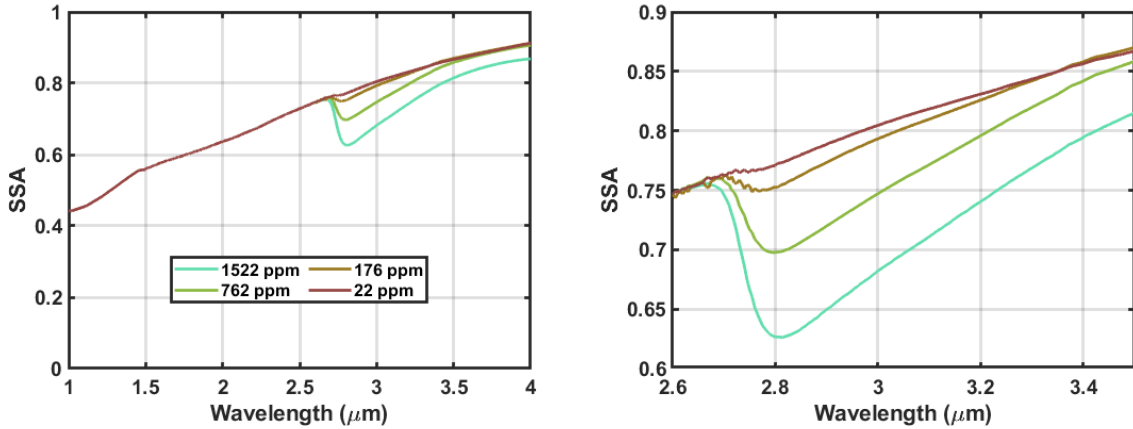


Figure S6. Derived single scattering albedo (SSA) for MORB glass spectra using the Hapke radiative transfer model.

We interpolated the data from the four experimental SSA spectra to create MORB spectra at 1 ppm total water intervals. For each wavelength, we calculated the ESPAT, defined as $(1-\omega)/\omega$ as a function of total water content. We then performed a linear fit to the experimental data. An example for a wavelength of 2.8 μm is shown in Figure S7. By using the linear fits at each wavelength, synthetic spectra were generated over the entire wavelength range and total water abundance range. Figure 2 in the main text shows a selection of the interpolated MORB spectra. We note the linear fit is not perfect, and the slight difference in the experimental data point and linear fit at 1522 ppm was the primary source of the mean error in total water retrievals.

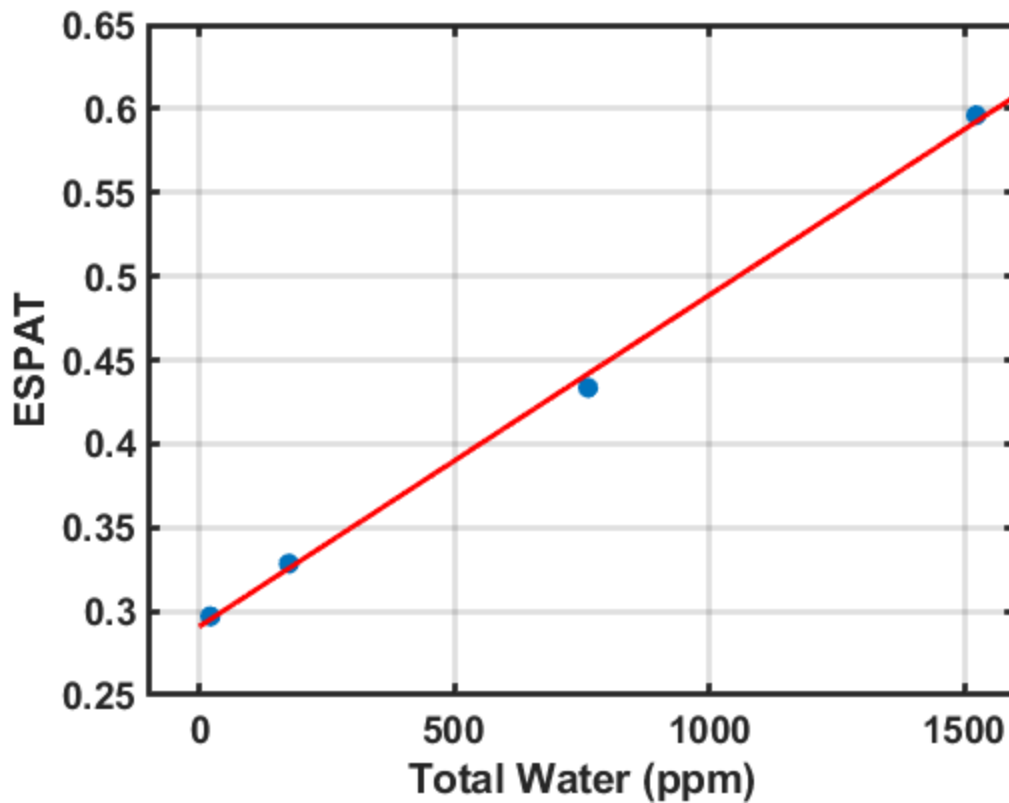


Figure S7. Linear interpolation method for hydrated MORB spectra. The blue dots are the ESPAT values calculated from the step-wise heating SSA spectra. The red line denotes a linear fit.

Synthetic Lunar Glass Spectra

The synthetic lunar glass spectra (orange and yellow glasses, (Wetzel et al., 2015)) were retrieved from the RELAB database. Two different datasets were needed to cover the 1 to 4 μm spectral range. We stitched the two datasets together by normalizing the reflectance values of the low-wavelength data to that of the high-wavelength data at 1.6 μm via division. Figure S8 shows the combined orange and yellow synthetic lunar glass spectra in laboratory reflectance geometry. The difference in band shape can be seen here. The orange glass has a band minimum at a slightly longer wavelength than the yellow glass and the MORB glass, which is relevant for the retrieval error as discussed in the main text. We then used the Hapke radiative transfer modeling used for the rest of the endmember spectra to convert between the RELAB geometry and SSA. The SSAs were used in spectral mixtures in the place of the MORB glass and converted into zero-phase reflectance measurements.

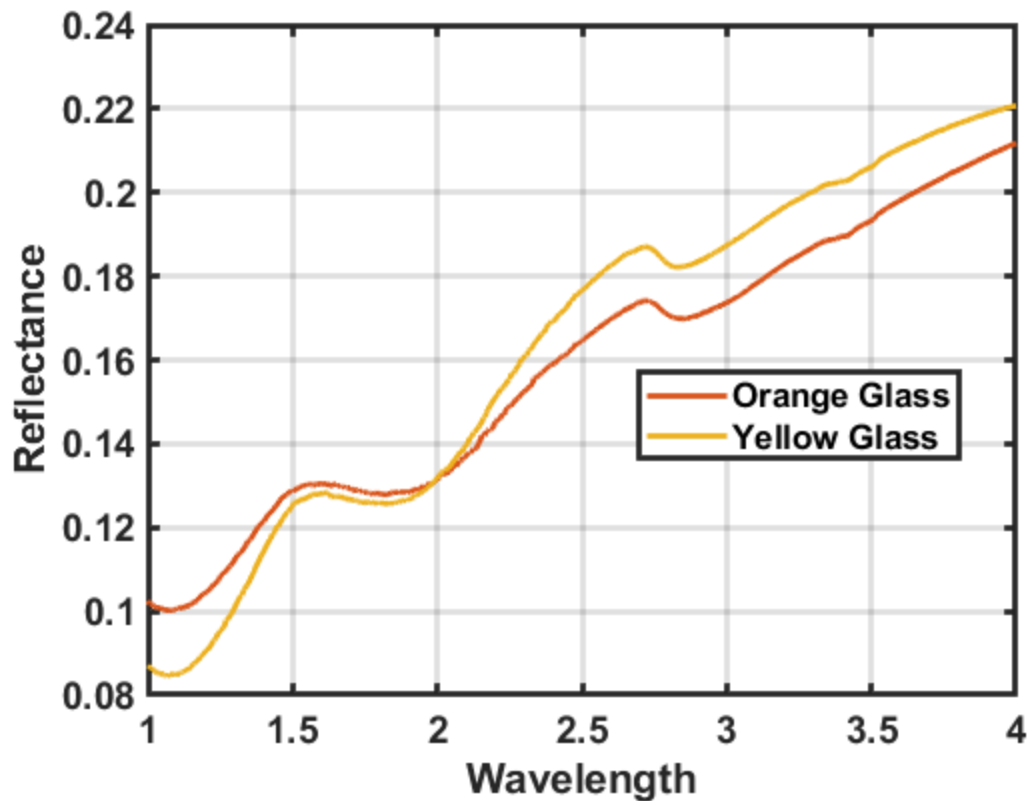


Figure S8. Reflectance spectra from the RELAB database of orange (OGV-5) and yellow (YG-5) synthetic glasses.

Band Depth Effects due to Pyroxene

The effects of pyroxene on the 3 μm band depth are discussed at length in the main text. Here we show one example of the effect from the simulations used to create Figure 8. For these simulations only, the interpolated MORB spectrum and MORB abundance were fixed at 1000 ppm and 0.3 respectively. Thus, each mixture here has 300 ppm total water, with only the amounts of pyroxene and regolith endmembers being varied. Here the spectra are shown with no noise added to the reflectance to clarify the band depth differences. We fit a linear continuum to the spectra using anchor points at 2.65 μm and 3.5 μm . The spectra and continua are shown in the left-hand side of Figure S9 for a mare mixtures with high pyroxene (31%) and a mare mixture with low pyroxene (12%). On the right it can be seen that the high-pyroxene mixture shows a deeper band than the low-pyroxene mixture. This highlights the care necessary in interpreting spectral band depths in the presence of pyroxene that may affect the continuum and affect the overall albedo.

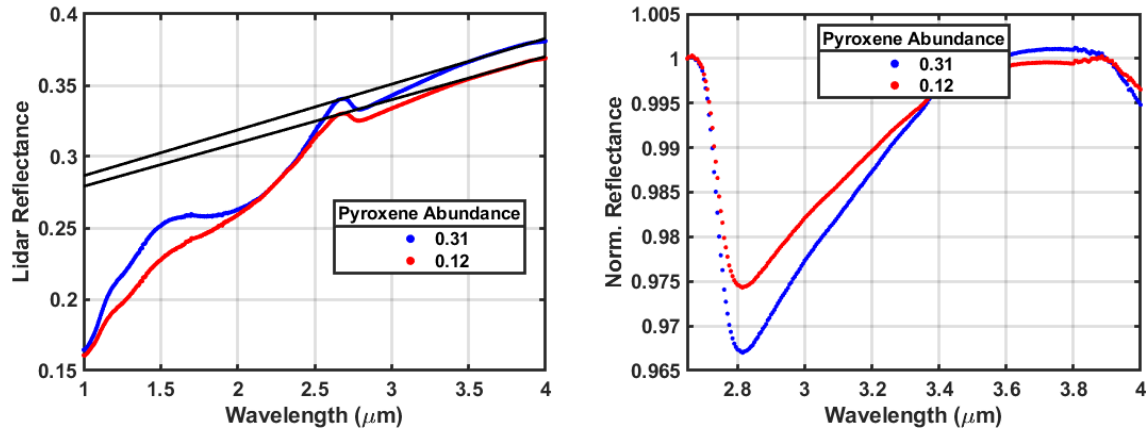


Figure S9. Example spectra, both with 300 ppm total water abundance, highlighting the effects of pyroxene on the observed band depth. These spectra were 2 of the 2000 spectra used to create Figure 8 in the main text, although for Figure 8 random noise was added to simulate the measurement SNR of 250.

Converting Total Water Abundance Error to Band Depth Error

The maximum standard deviation of total water error for our simulations was 52 ppm for the mare dataset. We converted this to a band depth precision to determine how well our multispectral lidar might constrain the 3 μm band depth. In the same manner as the pyroxene tests, we fixed the total water abundance at 52 ppm and generated 1000 noise-free mare spectra to determine the band depth for this abundance. Here we define band depth for the lidar as the difference between a linear continuum with anchor points at 2.65 and 3.5 μm and the reflectance spectrum at 2.8 μm. This ensures a band depth of zero when no hydration is present. The relative band depth is the continuum-removed band depth divided by the reflectance value at 2.65 μm. Two example spectra with 52 ppm and the continua for each are shown on the upper left in Figure S10. The continuum-removed 3 μm region is shown on the upper left of this figure. A histogram of the band depths from the 1000 spectra is shown on the bottom of Figure S10. The range in band depths comes from the different pyroxene and regolith abundances in the mixtures. The mean band depth value was 0.62%.

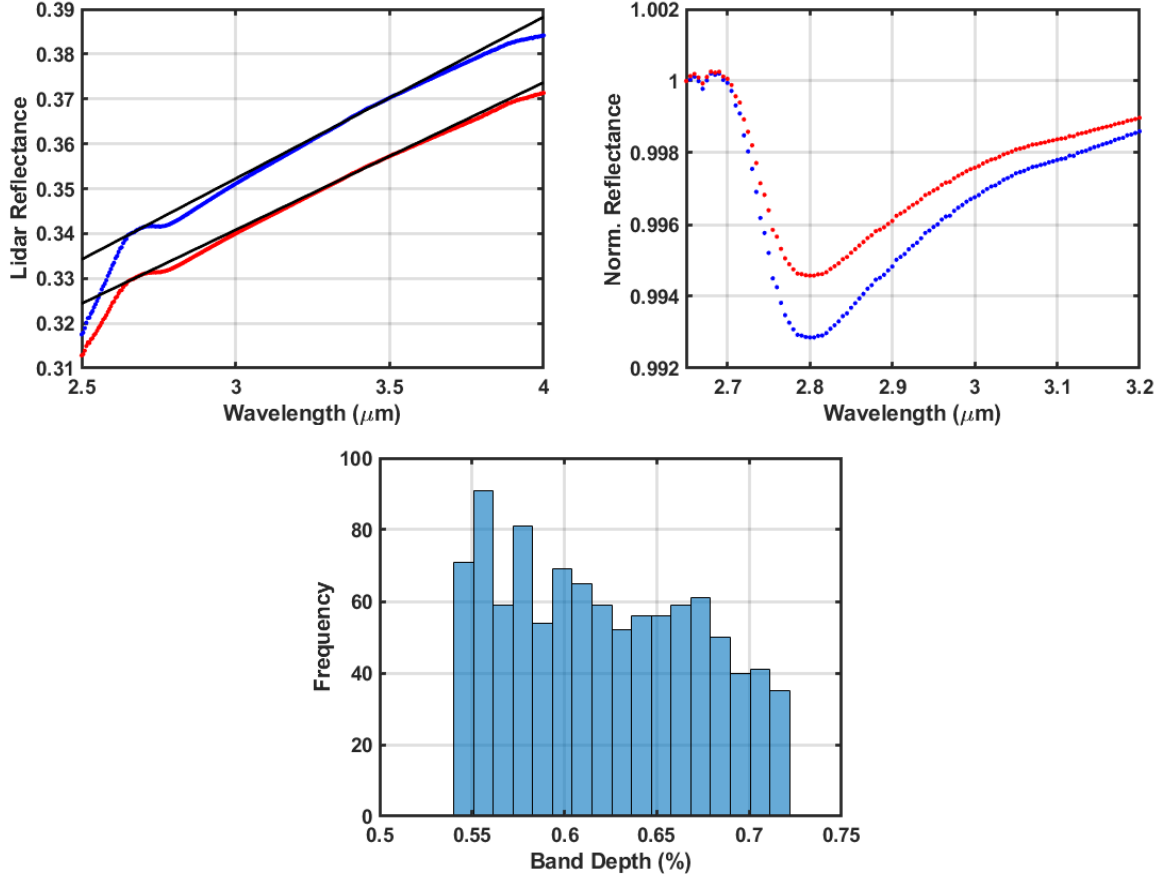


Figure S10. (Upper left) Two example spectra from the 52 ppm experiments. Black lines denote the linear continua used to calculate the band depth. (Upper right) Continuum-removed and normalized spectra. (bottom) Histogram of relative band depths (in percent) for the 52 ppm mare simulations (1000 spectra total). Each bin is 0.01% wide. The range of band depths comes from the difference in albedo of the continuum, which affects the relative band depth.

Multispectral Lidar Signal to Noise Ratio (SNR) Calculation

To determine the retrieval accuracy for a mid-infrared multispectral lidar we needed nominal instrument parameters to determine an instrument SNR. The precision of the multispectral lidar reflectance measurements is inversely proportional to the SNR of the instrument. For a pulsed lidar using waveform capture and photon counting, the SNR equation for a single lidar wavelength is given as (Sun, 2017):

$$SNR_{\lambda 1} = \frac{n_{signal} T_{int}}{\sqrt{T_{int} (n_{signal} + D(n_{dark} + n_{bkg}))}} \quad (S1)$$

Where n_{signal} is the average number of detected signal photons per second for that laser wavelength, T_{int} is the measurement integration time in seconds, D is the laser duty cycle

(fraction of the time the laser pulse is emitted), n_{dark} is the average number of dark counts per second, and n_{bkg} is the number of detected background photons per second.

The detected signal photon rate is calculated by:

$$n_{sig} = \frac{E_{Tx}}{hf} \cdot PRF \cdot \frac{\rho}{\pi} \cdot \frac{A}{R^2} \cdot T_A^2 \cdot \eta_R \cdot \eta_{det} \quad (S2)$$

Where E_{Tx} is the transmitted laser pulse energy, hf is the photon energy, PRF is the pulse repetition frequency of the laser (number of laser pulses per second), ρ is the normal albedo (surface reflectance at zero phase), A is the receiver aperture area in meters, R is the range from the lidar to the surface in meters, T_A is the one-way atmospheric transmission to the surface, η_R is the receiver optics transmission, and η_{det} is the detector efficiency (quantum efficiency and fill factor). The background photon rate is calculated by:

$$n_{bkg} = \frac{I_{solar}}{hf} \cdot \Delta\lambda \cdot \rho \cdot \left(\frac{FOV}{2}\right)^2 \cdot A \cdot T_A^2 \cdot \eta_R \cdot \eta_{det} \quad (S3)$$

Where I_{solar} is the solar spectral irradiance in units of $W/m^2/\mu m$ at the laser wavelength, $\Delta\lambda$ is the receiver spectral bandwidth in μm , FOV is the full-angle receiver field of view in radians. For a lunar orbital lidar the background signal contains contributions from solar reflected light (for sunlit terrain) as well as thermal photons emitted from the surface. At wavelengths near $3 \mu m$ it is particularly difficult to discriminate between thermal emitted photons and reflected solar photons as their contributions are similar in magnitude for the sunlit moon at low latitudes. As the lidar measurement is made using laser photons in a nominally nadir-pointing geometry, with the solar reflected and thermally emitted photons acting as noise, this technique has the distinct advantage of not requiring precise correction for the surface temperature or phase angle effects. In practice, the background photon contribution is removed in post-processing by averaging the detected signal between laser pulses. The number of dark counts per second (n_{dark}) is often determined experimentally for the detector of interest. The instrument parameters used to estimate the SNR are given in Table S2.

Table S2. Multispectral lidar instrument parameters for SNR calculation.

Instrument Parameter	Value	Rationale
Range	50 km	LRO science orbit mean altitude (Smith et al., 2010)
Receiver aperture diameter	25 cm	Reflective telescopes on orbital lidars (MOLA, GLAS, GEDI)
Receiver field of view (FOV)	1 mrad	
Normal Albedo	0.5	Average of Mare and Highlands spectra at $3 \mu m$

Surface temperature	385 K	Equatorial temperatures at noon
Laser pulse energy and PRF	100 μ J at 100 Hz	Demonstrated MIR intracavity OPO performance (Li et al., 2017)
Integration time	1 s	1.6 km along-track resolution
Receiver optics transmission	60%	Includes losses due to mirrors and lenses, bandpass filter
Receiver optical bandwidth	3 nm	Bandpass filter width
Detector dark current	250 kHz	HgCdTe APD dark count rate from (Sun et al., 2019)
Detector efficiency	65%	HgCdTe APD efficiency from (Sun et al., 2019)

Using Equations S1 through S3 and the values in Table S2, we calculated the multispectral lidar SNR over the range of lidar wavelengths (2 to 3.5 μ m). The results are shown in Figure S11. For the purposes of the performance simulations, we assumed a conservative estimate of an SNR of 250 for each lidar wavelength. Similar results for this design are described in (Cremons et al., 2020).

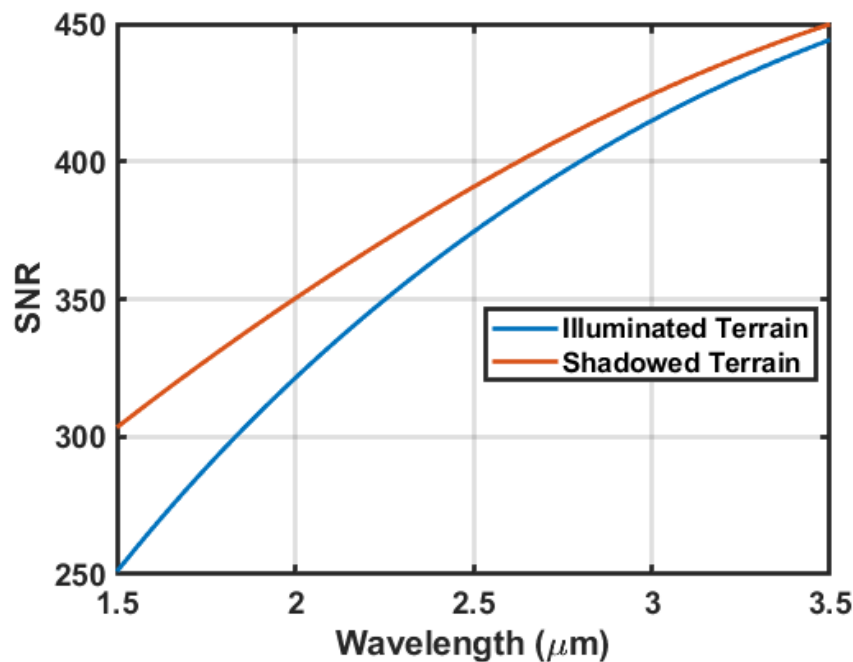


Figure S11. Multispectral lidar SNR calculation results for illuminated (385 K) and shadowed (110 K) terrain.

References

- Honniball, C. I., Lucey, P. G., Ferrari-Wong, C. M., Flom, A., Li, S., Kaluna, H. M., & Takir, D. (2020). Telescopic Observations of Lunar Hydration: Variations and Abundance. *Journal of Geophysical Research: Planets*, 125(9), e2020JE006484. <https://doi.org/10.1029/2020JE006484>
- Ichimura, A., Zent, A., Quinn, R., Sanchez, M., & Taylor, L. (2012). Hydroxyl (OH) production on airless planetary bodies: Evidence from H⁺/D⁺ ion-beam experiments. *Earth and Planetary Science Letters*, 345, 90–94.
- Li, S. X., Yu, A. W., Sun, X., Fahey, M. E., Numata, K., & Krainak, M. A. (2017). A multi-wavelength IR laser for space applications. *Laser Radar Technology and Applications XXII*, 10191, 101910L. <https://doi.org/10.1117/12.2262391>
- Lucey, P. G., Petro, N., Hurley, D., Farrell, W., Prem, P., Costello, E., Cable, M., Barker, M., Benna, M., Dyar, D., & others. (2021). Volatile interactions with the lunar surface. *Geochemistry*, 125858.
- McCord, T. B., Taylor, L. A., Combe, J.-P., Kramer, G., Pieters, C. M., Sunshine, J. M., & Clark, R. N. (2011). Sources and physical processes responsible for OH/H₂O in the lunar soil as revealed by the Moon Mineralogy Mapper (M3). *Journal of Geophysical Research: Planets*, 116(E6). <https://doi.org/10.1029/2010JE003711>
- Smith, D. E., Zuber, M. T., Jackson, G. B., Cavanaugh, J. F., Neumann, G. A., Riris, H., Sun, X., Zellar, R. S., Coltharp, C., Connelly, J., Katz, R. B., Kleyner, I., Liiva, P., Matuszeski, A., Mazarico, E. M., McGarry, J. F., Novo-Gradac, A. M., Ott, M. N., Peters, C., ... Zagwodzki, T. W. (2010). The lunar orbiter laser altimeter investigation on the lunar reconnaissance orbiter mission. *Space Science Reviews*, 150(1–4), 209–241. <https://doi.org/10.1007/s11214-009-9512-y>

- Starukhina, L. V., & Shkuratov, Y. G. (2010). *Simulation of 3- μ m Absorption Band in Lunar Spectra: Water or Solar Wind Induced Hydroxyl?* 1385.
<https://ui.adsabs.harvard.edu/abs/2010LPI....41.1385S>
- Sun, X. (2017). Lidar sensors from space. In *Comprehensive Remote Sensing* (pp. 412–432).
<https://doi.org/10.1016/B978-0-12-409548-9.10327-6>
- Sun, X., Abshire, J. B., Krainak, M. A., Lu, W., Beck, J. D., Sullivan, W. W., Mitra, P., Rawlings, D. M., Fields, R. A., Hinkley, D. A., & Hirasuna, B. S. (2019). HgCdTe avalanche photodiode array detectors with single photon sensitivity and integrated detector cooler assemblies for space lidar applications. *Optical Engineering*, 58(6), 067103. <https://doi.org/10.1117/1.oe.58.6.067103>
- Sunshine, J. M., Farnham, T. L., Feaga, L. M., Groussin, O., Merlin, F., Milliken, R. E., & A'Hearn, M. F. (2009). Temporal and Spatial Variability of Lunar Hydration As Observed by the Deep Impact Spacecraft. *Science*, 326(5952), 565–568.
<https://doi.org/10.1126/SCIENCE.1179788>
- Wetzel, D. T., Hauri, E. H., Saal, A. E., & Rutherford, M. J. (2015). Carbon content and degassing history of the lunar volcanic glasses. *Nature Geoscience*, 8(10), 755–758.
<https://doi.org/10.1038/ngeo2511>