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2022 PSIDA

Identifying Planetary Materials

by Combining a custom Mineralogical Database with Machine Learning based Multi-Spectral Classification

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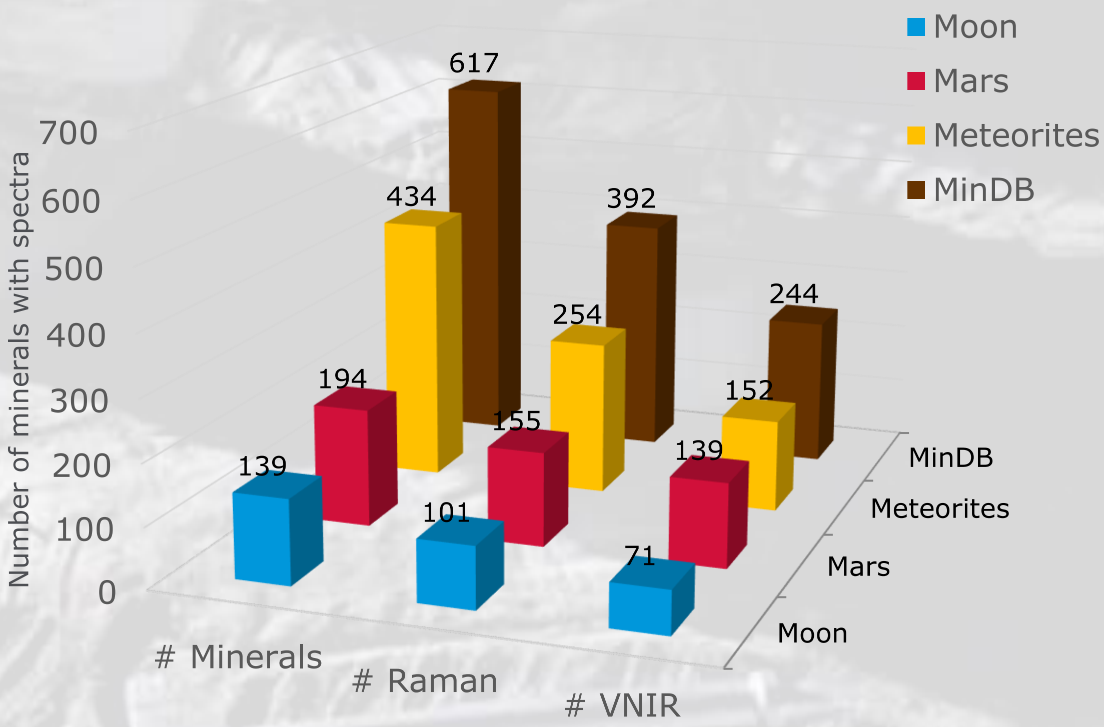
Analytical Toolset for Surface Explorations

Preliminary recognition of minerals or chemical compositions immediately available to Science Backroom

PANGAEA Mineralogical Database

1. Based on Bibliographic research:
   - **Catalog** of all currently known minerals on Moon, Mars, Meteorites
2. Based on available archives and our measurements:
   - **Archive** of reference spectra of minerals and their mixtures



Mineralogical Catalogue: Minerals / Endmembers

Name of mineral → Formula → Group → Spectral Detectability → Description → References

Name	Formula	Group	Subgroup1	Subgroup 2	Structural groupname	# Raman spectra	Raman Detection	# VNIR spectra	VNIR Detection
Acanthite	Ag_2S	Sulfides			Acanthite	2			
Actinolite / Actinote / Actynoli	$\{Ca_2\}\{Mg_{4\cdot5-2\cdot5}Fe_{0\cdot5-2\cdot5}\}(Si_8O_{22})(OH)_2$	Silicates	Inosilicates	Amphibole	Amphibole	115	0.9	115	0.5
Addibischoffite	$Ca_2Al_6Al_6O_{20}$	Oxides	Metal Oxides	Sapphirine	Sapphirine				
Adrianite	$Ca_{12}(Al_4Mg_3Si_7)O_{32}Cl_6$	Silicates	Nesosilicates	Wadalite					
Aegirine / Aegirite	$NaFe^{3+}Si_2O_6$	Silicates	Inosilicates	Clinopyroxene	Pyroxene	50	0.9	*19*	0.1
Aenigmatite / Cossyrite	$Na_4[Fe^{2+}{}_{10}Ti_2]O_4[Si_{12}O_{36}]$	Silicates	Inosilicates	Aenigmatite	Sapphirine	28			
Ahrensite	$SiFe_2O_4$	Silicates	Nesosilicates	Spinel	Spinel				
Akaganeite / Akaganéite	$(Fe^{3+},Ni^{2+})_8(OH,O)_{16}Cl_{1.25}\cdot nH_2O$	Oxides	Hydroxides		Coronadite	1		7	

- 617 minerals in total
- Endmembers and Intermediate (Compositions)
- Over 600 references

MinDB: Analytical datasets

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Reference Spectroscopic archives

Molecular
- **VNIR/SWIR** reflection
- **Raman** scattering

Atomic
- LIBS emission
- XRF fluorescence

Informations about
- mineralogy
- chemical abundances
- mixtures

~10,000 High Quality Raman & VNIR Spectra of planetary analog minerals

Open Access Databases:
- VNIR: USGS science for a changing world, RELAB, ECOSTRESS
- Raman: RRUFF

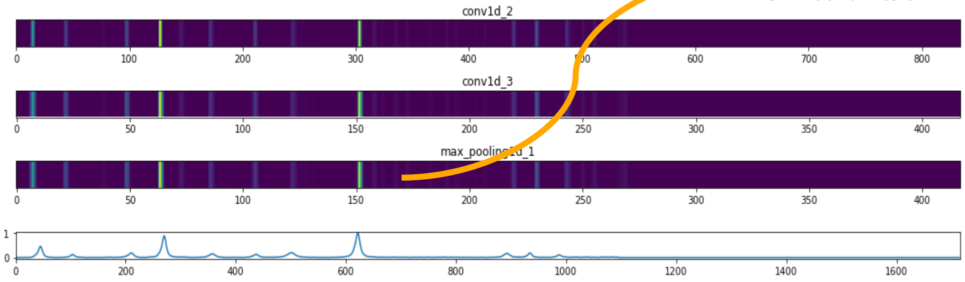
Our own spectroscopy

Samples from:
- Mineralogical Museum Bonn
- GeoMuseum Cologne
- Mineralogische Staatssammlung Munich
- PANGAEA Sites: Ries Crater, Lanzarote

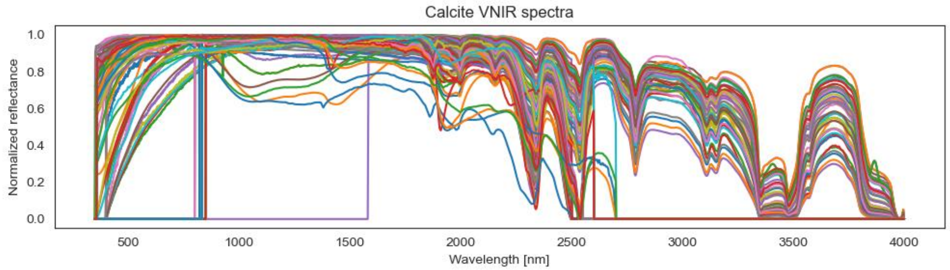
Comparison and validation of spectra

Detection of characteristic spectral features

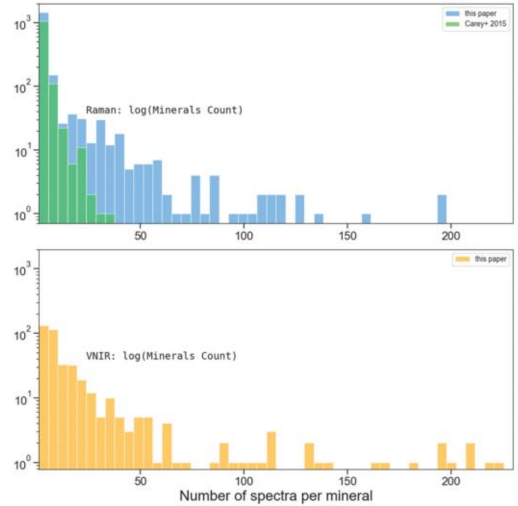
1. Calcite: 76.15%
2. Aragonit: 12.80%
3. Dolomit: 12.05%



Large variation in quaility & wavelength ranges of available spectra

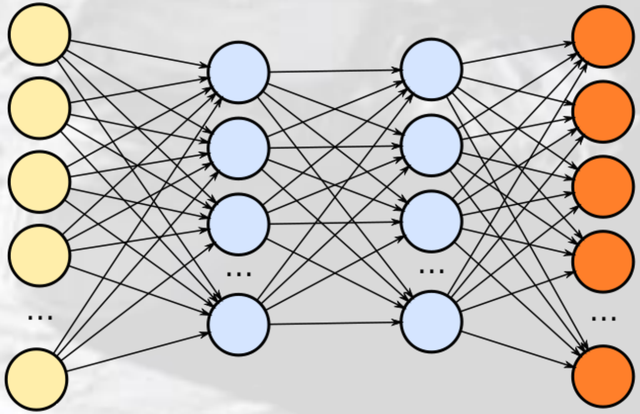


Not enough representative data
→ Augmentation & Balancing



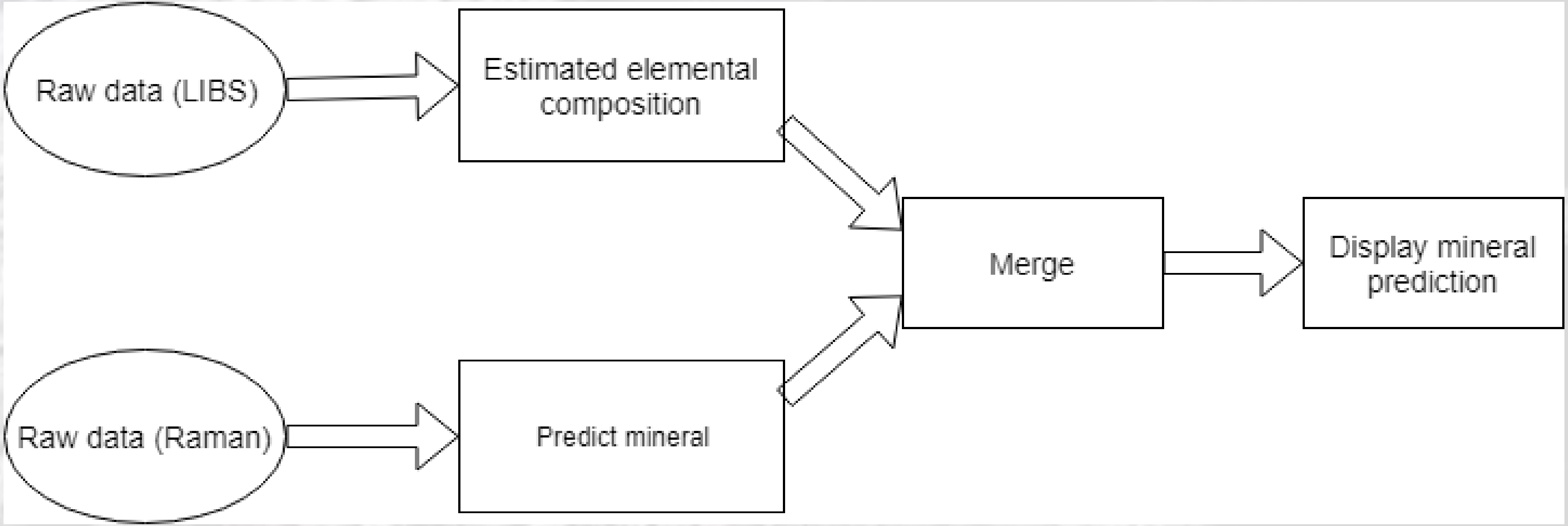
Drozdovskiy, I. et al. 2020, Data in Brief, 31, 105985.

Recognition: Machine Learning approach?



- Benefits:
  - Fast & Accurate to match
  - Handles multi-variety of data
  - Self-Learning improvements from New Data!
- Drawbacks
  - Requires Massive Data sets
  - Needs to teach algorithms from the data

Novel approach: 2-types of Data Fusion

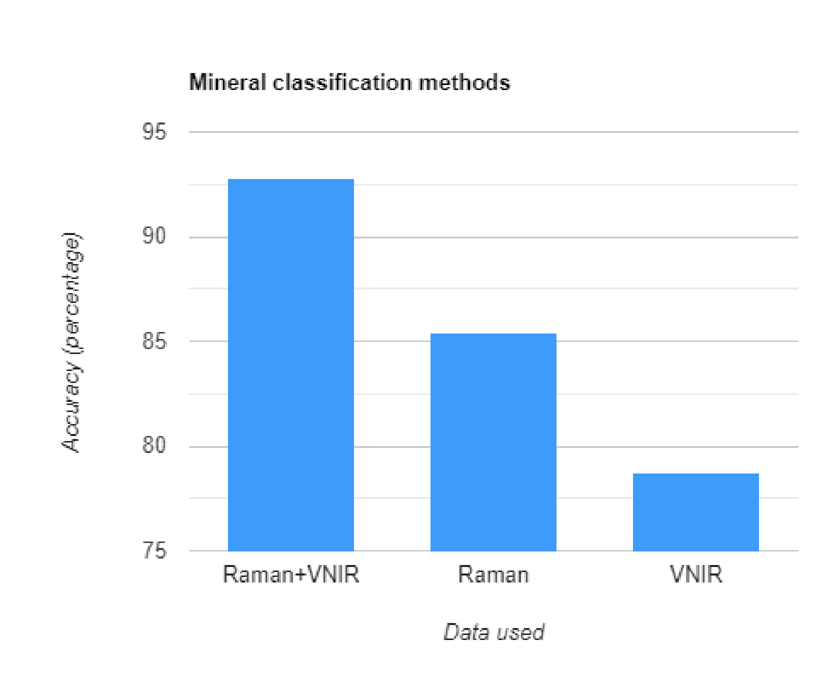


- Combining data from different spectroscopic methods

Reliable identification of minerals

- **Improved** the current state-of-the-art matching algorithm for *single spectroscopic method* with our Deep Convolutional Neural Network solution

- Classification based on *dual Raman+VNIR, Raman+LIBS or VNIR+LIBS* **outperformes the state-of-the-art** mineral classification based on single method



Jahoda, P., Drozdovskiy, I., Payler, S.J., Turchi, L., Bessone, L. and Sauro, F., 2021. Machine learning for recognizing minerals from multispectral data. Analyst, 146(1), pp.184-195.

Multi-label Recognition: Mineral Mixtures

The goal: to choose a suitable algorithm to identify components (individual minerals) in a combined spectra of mineral mixtures

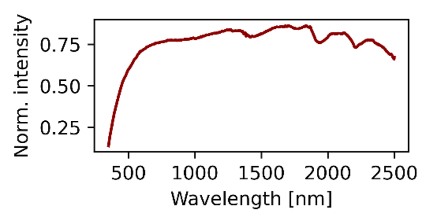
halite

muscovite quartz

opal pyrope alunite

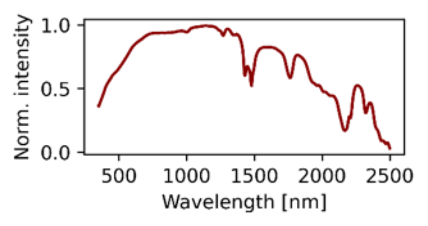
sulphur

quartz



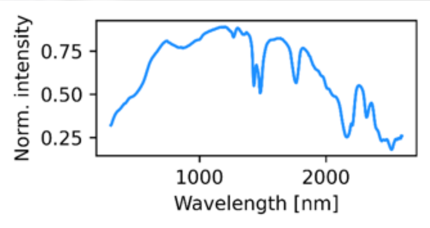
OR

alunite



Multi-class classification

alunite AND quartz



NEW! Multi-label classification

→ Recognizing Planetary Rocks And Minerals

Combining a Custom Mineralogical Database with Machine Learning based Multispectral Unmixing

617 minerals

Spectral coverage by method

64.12% Raman

41.59% VNIR

~10^4 spectra

Spectral coverage by prominence

69.84% Meteorites

33.62% Mars

24.09 % Moon

Petrographic catalogue & Custom archive of reference spectra

Developed and tested together in the context of ESA's astronaut field science training using analogue environments, PANGAEA, the mineral library and recognition software are a real-time decision support tool for future planetary surface exploration missions.

Metrics are stored in the database for continuous improvement

LIBS & XRF

Raman & VNIR

Deep learning for mineral classification

Elemental composition estimation

Prediction fusion & Spectral Unmixing

Prediction accuracy per method

92.76% Raman & VNIR

83.21% Raman & LIBS

79.34% VNIR & LIBS

- Mineralogical DataBase – Data in Brief
  https://doi.org/10.1016/j.dib.2020.105985
- Machine Learning – The Analyst
  https://doi.org/10.1039/D0AN01483D

Field Analytical Tools for Exploration

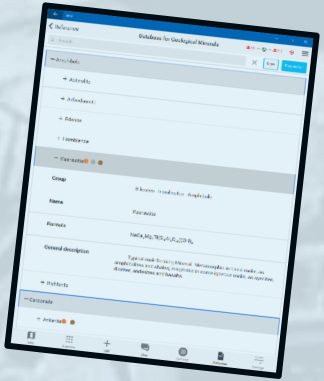
Mineralogical Database

EFB

Catalog of Planetary Analog Minerals

Spectral Libraries

Software to Match Spectra to Minerals



Combined Handheld Spectrometers

Science Support