

COLLECTION OF CASE STUDIES: HOW MUCH OF THE PUZZLE CAN WE SEE?

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on behalf of the RDA Sample Type Classification Working Group



SAMPLE TYPE CLASSIFICATION

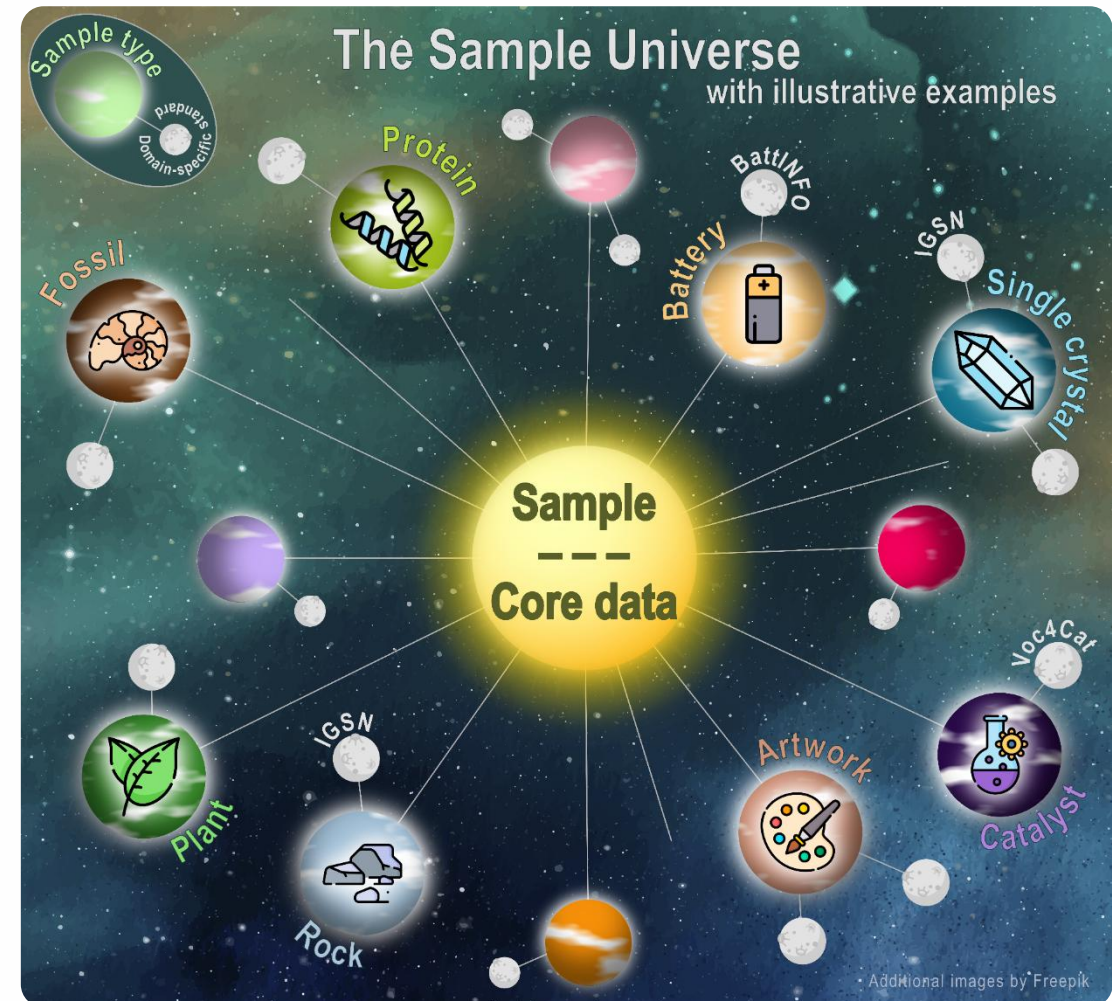
Guide the metadata in the right direction

A standardised top-level classification of Sample Types:

- Every sample is assigned a **Type**
- Each Type points to appropriate **existing** standards
- Enables early identification of what metadata to capture

Key characteristics:

- Does **not replace** domain-specific vocabularies, rather **connects** them
- Improves **completeness and relevance** of sample metadata
- **Broad but shallow:** Types act as entry points, not detailed descriptions



STEP ONE: KNOW YOUR SAMPLE LANDSCAPE

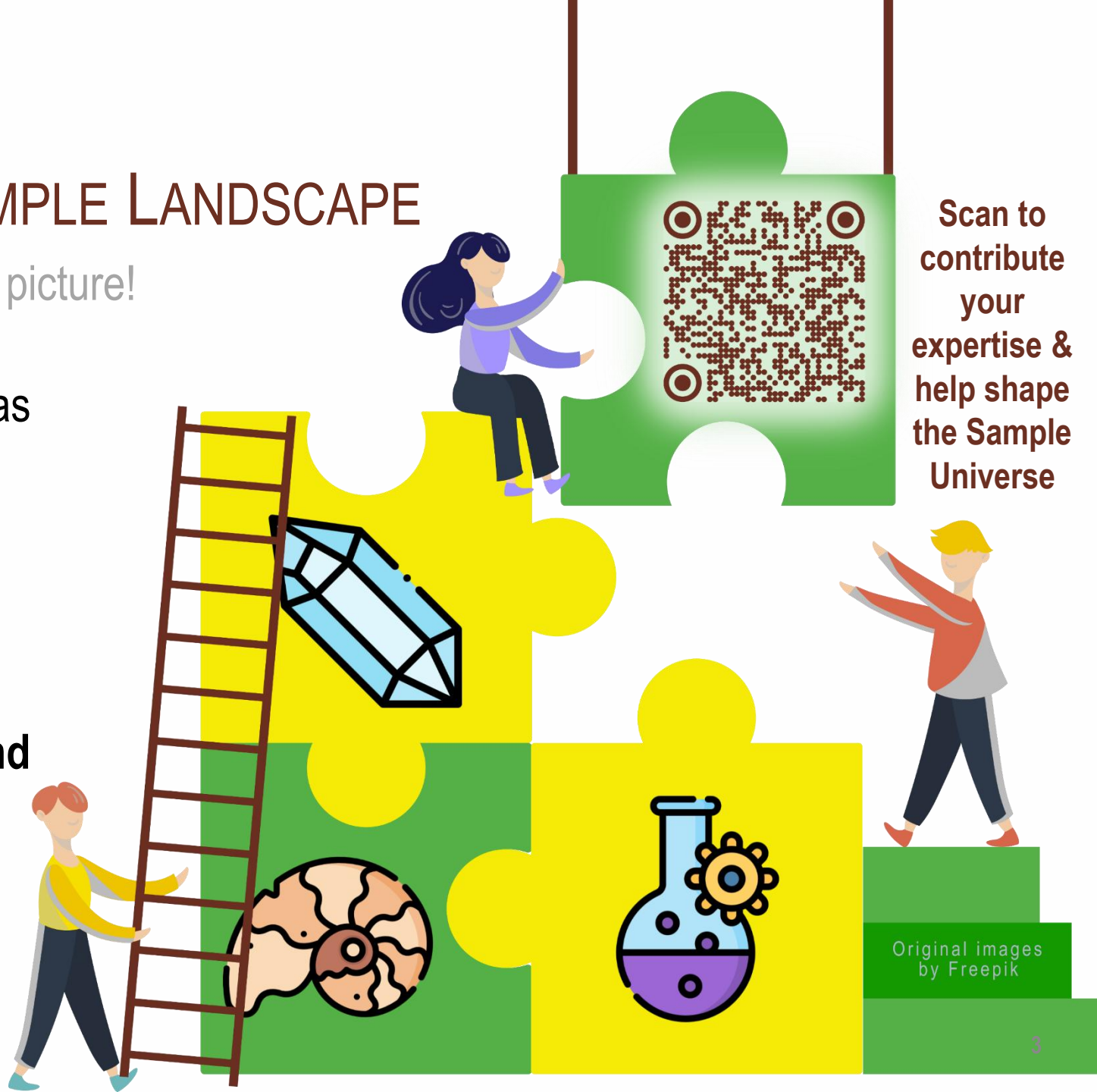
Add YOUR piece to the bigger picture!

We are collecting Case Studies from as many domains as possible, asking for:

- Basic sample description
- Characteristic properties
- Existing standards

We need the expertise of you and your facility users

Scan the QR code, or visit
<https://github.com/RDA-Sample-Type-Classification-WG/Case-Studies>



Scan to contribute your expertise & help shape the Sample Universe

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THE PICTURE SO FAR

Domains

- Condensed Matter Physics - magnetism
- Magnetism and (many-body) Quantum Phenomena
- Polar Science
- Material Science
- Marine Geology and Environmental Sciences
- Marine Research
- Liquid Samples
- Soft and Biological Matter
- Neutron Scattering
- Geochemistry
- Photovoltaic Materials
- Synchrotron Physical Sciences
- Archaeology

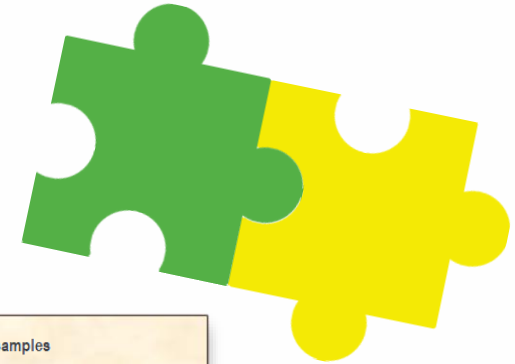


THE PICTURE SO FAR

Samples



- Single crystals
- Metal-organic perovskites
- Ice cores
- Rocks
- Extraterrestrial materials
- Pottery
- Polymer molecules
- Glass
- Nanoscale systems
- ...



Marine sediment core samples		
Biological samples - whole organisms <i>Examples: Individual fish</i>	Fluid inclusions	
Biological samples - partial <i>Examples: scales, fin clips</i>	Synthetic materials <i>Examples: glasses, petrology</i>	Glass
Non-biological samples <i>Examples: water, sediment</i>	Protein powders	Soil
Vessels <i>Examples: fishing boat, resin</i>	Proteins dissolved in water	Complete objects and fragments (as found)
Pure liquids	Phospholipid membranes in water	Cuts/selected fragments
Mixtures of liquids	Polymer molecules	(Thin) sections
Solutions of substances in liquids	Thin film devices	Powders and drillings
Glasses	Ephemeral samples <i>Examples: thin films during growth to experiment, can be destroyed during measurement</i>	Molecular tracers <i>Examples: aDNA, proteins</i>
Inorganic crystalline materials <i>Examples: single crystals, powders</i>	Continuous samples <i>Examples: liquids, gases; individual samples, some quantity of the whole</i>	Polycrystalline (powder) samples
Nanostructured materials	Unique samples <i>Examples: one-off archaeological artifacts, engineering structures</i>	Single crystals
Nanoscale systems	Geological materials <i>Examples: stones</i>	Thin films
Rocks	Biogenic materials <i>Examples: wood, bone, antler</i>	Polar sediments <i>Examples: marine, peat, lake cores</i>
Minerals	Pottery	Geological specimens <i>Examples: land, dredge, fossils</i>
Extraterrestrial materials	Metals and metallurgical by-products <i>Examples: slag</i>	Ice cores
Soils/regolith		Herbarium specimens
Fluids <i>Examples: groundwater</i>		Biological samples <i>Examples: marine pelagic and benthic, mammals, birds</i>
		Elemental metals
		Metal alloys
		Oxide ceramics
		Metal-organic perovskites



THE PICTURE SO FAR

Properties

Common Properties

- Physical state *single crystal, powder, thin film, gel, liquid*
- Physical parameters *dimensions, volume, shape, mass, internal structure, age*
- Processing, treatment, preparation *chemical treatments, physical changes (e.g. crushing)*
- Collection/creation location *geographical area, lat/long, type of environment, laboratory, supplier*
- Personnel *PI, collector or creator*
- Classification *biological taxonomy, classes of magnetism*



Multi-domain Properties

- Sample subsection/granularity
- Biological descriptors (sex, maturity)
- Magnetic ground state, temperature
- Chemical & crystal composition
- ...

*Earth & environment
Biological sciences
Materials sciences
Experimental techniques*

Domain-specific Properties

- Efficiency *Photovoltaic Materials*
- Relation to human activity *Archaeology*
- Hydrogen presence *Neutron Scattering*
- Vessel activity *Marine Research*
- ...



THE PICTURE SO FAR

Vocabularies & Standards

Earth & environment sciences and Archaeology

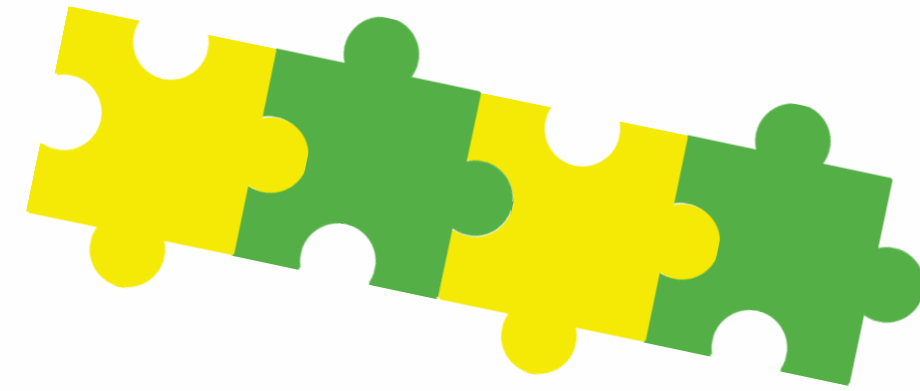
have a large array of standardised terminologies to describe different aspects of samples

Materials sciences

have some limited standardisation

Other domains

none reported: EITHER no such vocabularies OR they have yet to be widely adopted



Very little crossover, even between closely related fields

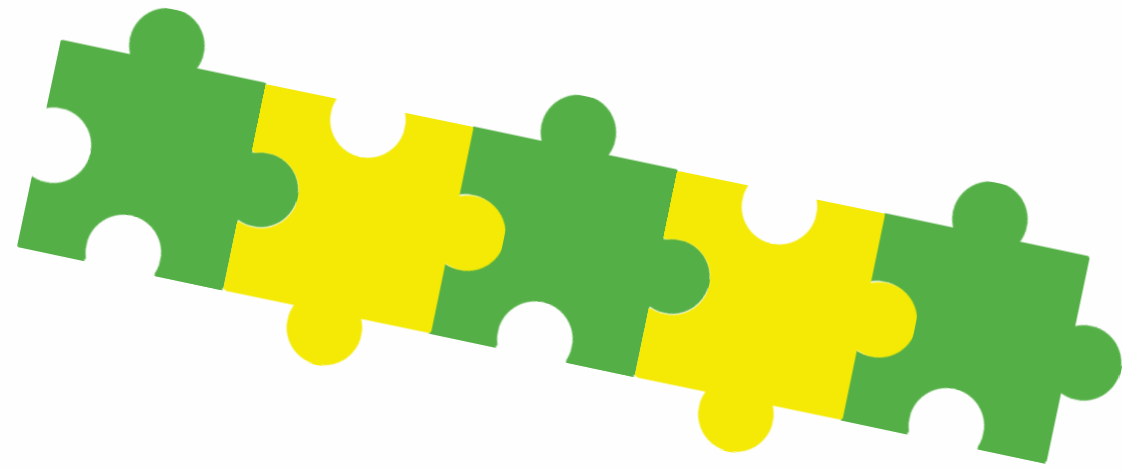
Many vocabulary hosting services are domain-specific

Rapidly expanding area – many recently developed or under initial development



THE PICTURE SO FAR

Persistent Identifiers



Out of 13 responses, 10 said they don't use PIDs



IGSN



ORCID



The remaining 3 identified:

- IGSN (samples, through DataCite)
- ORCID (people)
- ROR (institutes)

NEXT STEPS: UP FOR DISCUSSION

Building a vocabulary

Goal: develop a recommendation for one or more vocabularies for global, cross-domain classification of material sample types

Expanding the case studies: what else do we need to know?

Making data useful: how do we translate the case studies into a vocabulary?

Building the list: what sort of technical implementation would be most useful?

Finding the gaps: what else should we be thinking about?

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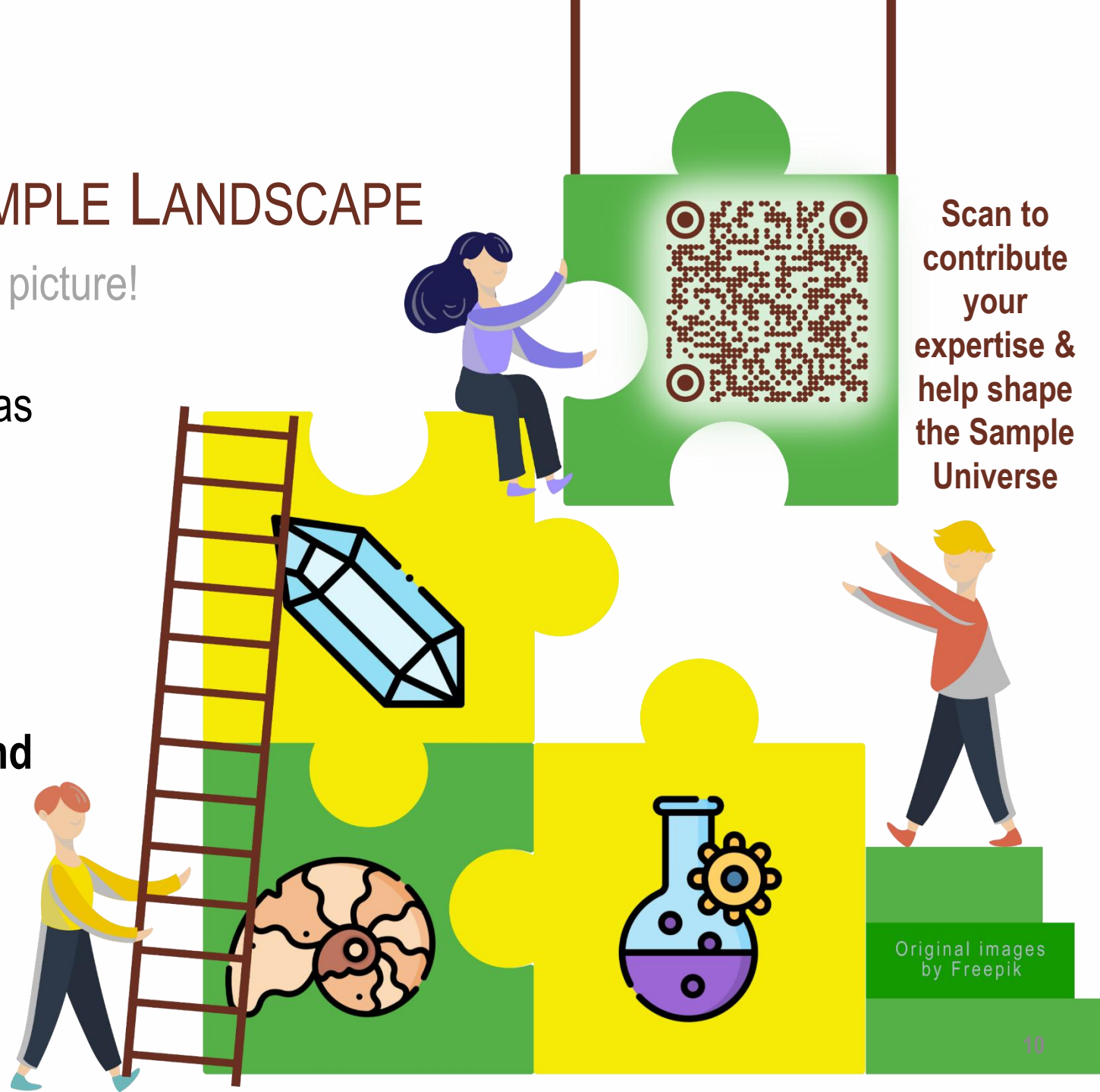
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