

POLYMERNEXUS - POLYMER KNOWLEDGE GRAPHS WORKFLOW FOR SEMANTIFICATION OF POLYMER DATASETS

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MOTIVATION

- Complex physical and chemical structures of synthetic rubber polymers
- Precise measurement of Polymer properties is critical for manufacturing high performance rubbers
- Tracking and understanding of the effect of Polymer properties is of utmost importance for the development of material models
- Enabling non-technical users to get insights from a Polymer Knowledge Graph is key to transforming raw data into actionable knowledge for innovation and decision-making.

CONTEXT

- Can we integrate Polymer datasets into a Knowledge Graph?
- Can we have consistent automated transformation of raw data based on conceptual models developed within InSuKa?
- Can domain experts have an intuitive user interface to query and understand the raw and vulcanized Polymer properties?
- Can the user interface be used by novices of Knowledge Graphs to query Knowledge Graphs?

POLYMERNEXUS AT A GLANCE



SHACL Shapes Based
Transformation of Raw
Polymer Datasets

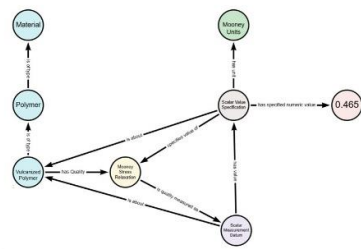


LinkML Universal Converter Box
for Automated SHACL Shapes
Generation from YAML Model

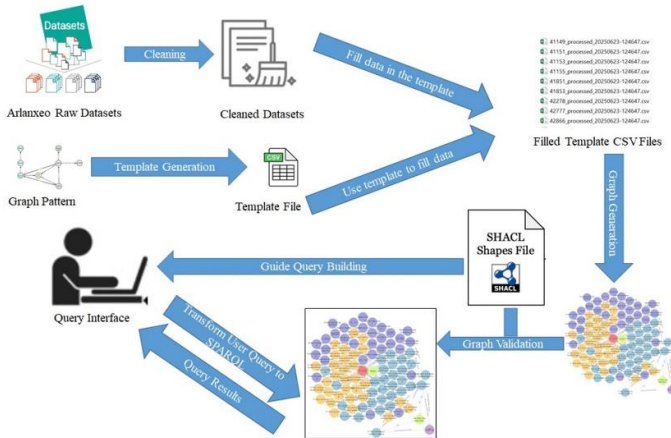


Flask based Web Application
for Seamless Data Transformation
and Retrieval

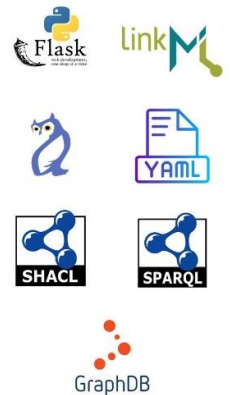
MEASUREMENT GRAPH PATTERN



ARCHITECTURE OF POLYMERNEXUS APPLICATION



INSIDE POLYMERNEXUS



How can the query interface help?

- Get all Vulcanized Compounds with Hardness mean value above 65
- Get all raw polymers which have Styrene Content in the range 10 to 20
- Get all raw Polymers with Vinyl content above 50 and Glass transition temperature below -20
- Get all Vulcanized compounds with maximum value for D Median
- Get all Vulcanized Compounds with minimum value for Mooney Stress Relaxation

FUTURE DIRECTIONS

- Integration of more datasets such as Mixing Recipes including Device and Ingredient Specifications
- Sub Graph Exploration based on user queries
- Visual Interface for Graphs showing relationships between Polymer Properties, Recipe, Device and Ingredient Specifications

SPARQL Query Builder

Query Template:

Property 1:

Comparison 1:

Value 1:

Property 2:

Comparison 2:

Value 2: