

# **Enhanced Streamlit LLM Knowledge Graph Generator**

Upload a PDF



Influence of Ionomer Content in the Catalytic Layer of MEAs.pdf 3.2MB

PDF content extracted successfully.

Executing Chunking Agent...

Download Chunking Agent Output

Total chunks created: 17

Executing Entity Extraction Agent...

Download Entity Extraction Agent Output

Final Extracted Entities:

To condense the provided information into a cohesive knowledge graph structure, we can organize the details under distinct categories, identifying key entities and their relationships. Here is how it can be structured:

# Material

- Ionomers and Polymers:
  - o Aquivion® PFSA Polymer
  - Nafion<sup>®</sup>
  - SSC Polymer
- · Catalysts and Alloys:
  - Platinum (Pt)
  - Platinum-Cobalt (PtCo)
  - o 50% Pt on Ketjenblack (Pt/KB)
  - o 50% PtCo on Ketjenblack (PtCo/KB)
- Membranes and Composite Materials:
  - Aquivion®-reinforced membrane R79-01SX+
  - o Aquivion® PFSA D79-25BS and D79-20BS
- Other Materials:
  - Ethanol
  - Water (H2O)
  - Cobalt nitrate
  - Ammonium carbonate
  - Ketjenblack EC

# Manufacturing

- Preparation Processes:
  - o MEA (Membrane Electrode Assembly) preparation
  - Electrode preparation
  - Catalytic ink preparation

- Hot pressing
- Methods:
  - o Deposition

## Measurement

- Characterization Techniques:
  - Electrochemical studies and characterization
  - o Transmission Electron Microscopy (TEM)
  - X-ray diffraction (XRD)
  - Scanning Electron Microscopy (SEM)
- Analyses:
  - o Electrochemical Surface Area (ECSA)
  - Steady-state galvanostatic measurements
  - Cyclic voltammetry (CV)

# **Property**

- Ionomer Properties:
  - Protonic conductivity: High
  - o Chemical stability: High
  - o Thermal stability: High
- Comparison with Nafion®:
  - o Crystallinity, Tg: Higher
  - o Swelling: Lower
- Physical Characteristics:
  - o Membrane thickness: 10 μm
  - o Equivalent weight of ionomer: 790 g/mol
- Crystallite and Particle Sizes:
  - o Pt in Pt/KB: Crystallite: 2.5 nm, Particle: 2.8 nm
  - o PtCo in PtCo/KB: Crystallite: 3.3 nm, Particle: 3.4 nm

## **Parameter**

- Operating Conditions:
  - o Temperature: 80-95°C
  - o Pressure: 1.5-2 bar abs
  - o Humidity: 50% RH
- Hot Pressing Conditions:
  - Temperature: 125 °C
  - Pressure: 20 kg/cm²
  - o Time: 5 min
- Measurement Conditions:
  - o Potential range: 20 to 1250 mV
  - Sweep rate: 50 mV/s

This organization illustrates relationships and dependencies among entities in the context, representing a structured approach to constructing a knowledge graph in materials science related to fuel cell technology.

Executing Relationship Extraction Agent...

Download Relationship Extraction Agent Output

Final Extracted Relationships:

Based on the extracted relationships from the provided data, the consolidated output is as follows:

## Manufacturing Inputs:

Critical materials and components like PSFA membrane, PGM catalysts, Aquivion®, Nafion®,
catalytic ink, Gas Diffusion Layer Sigracet-25BC, electrodes, R79-01SX+ membrane, catalyst
powder, CU grid, 2-propanol, Pt, and PtCo are identified as essential inputs in the manufacturing
process of fuel cell components.

## • Manufacturing Outputs:

 The process yields products such as membrane-electrode assemblies (MEAs), Pt/KB, and PtCo/KB.

## • Measurement Inputs:

• Electrocatalyst powders, Pt/KB, PtCo/KB, and MEA are utilized in performance measurements.

## • Measurement Outputs:

 Results include detailed analysis such as morphology, crystallographic structure, degree of alloying, crystallite sizes, polarization curves, mass activity (j m), and electro-kinetic parameters (ECSA, jm @ 0.9V IRfree).

## • Properties:

 Various characteristics such as catalyst powder, Pt loading, crystallite sizes, and commercial gas diffusion layer (Sigracet-25BC) are noted, alongside electrochemical surface area (ECSA), MEArelated parameters (ECSA, jm @ 0.9V IRfree).

#### · Parameters:

• Includes morphology, crystallographic structure, degree of alloying, potential, and sweep rate, which are critical for assessing and optimizing fuel cell performance.

To apply this information effectively in a materials ontology framework like EMMO, detailed information about each category from academic sources would be necessary, focusing on materials, manufacturing processes, measurements, and properties to draw specific conclusions and relationships.

Executing JSON Generation Agent...

input for agent ison

# SYSTEM INSTRUCTIONS

You are a Materials Science assistant specialized in building comprehensive knowledge graphs (KG) using the <a href="http://emmo.info/emmo#">http://emmo.info/emmo#</a> ontology, specifically in TTL or JSON-LD format.

## Your objectives:

- 1. Ignore any text or examples that appear outside the section labeled DATA: ... END DATA.
- 2. **Fully parse** each piece of data under DATA (including materials, manufacturing processes, measurements, properties, parameters).
- 3. Create instances for all relevant items, typed to the correct EMMO classes:
  - :EMMO\_4207e895\_8b83\_4318\_996a\_72cfb32acd94 → Material
  - :EMMO\_a4d66059\_5dd3\_4b90\_b4cb\_10960559441b → Manufacturing
  - :EMMO\_463bcfda\_867b\_41d9\_a967\_211d4d437cfb → Measurement
  - :EMMO\_b7bcff25\_ffc3\_474e\_9ab5\_01b1664bd4ba → Property
  - o :EMMO\_d1d436e7\_72fc\_49cd\_863b\_7bfb4ba5276a → Parameter
- 4. Link them with the correct object properties, respecting domain/range rules:
  - Material → is\_manufacturing\_input → Manufacturing (emmo:EMMO\_e1097637)
  - o Manufacturing  $\rightarrow$  has\_manufacturing\_output  $\rightarrow$  Material (emmo:EMMO\_e1245987)
  - o Material → is\_measurement\_input → Measurement (emmo:EMMO\_m5677989)
  - $\begin{tabular}{ll} \bullet & Measurement $\rightarrow$ has\_measurement\_output $\rightarrow$ Property (emmo:EMMO\_m87987545) \\ \end{tabular}$

12/30/24, 7:40 PM

- o Manufacturing → has\_parameter → Parameter (emmo:EMMO\_p46903ar7)

mini5 Material → has\_property → Property (emmo:EMMO\_p5778r78)

- 5. Output a complete JSON-LD knowledge graph with:
  - @context linking ex to http://example.com/ and emmo to http://emmo.info/emmo#.
  - graph array containing all individual nodes (for all data from DATA) and all edges/triples.
  - No commentary—only the final JSON-LD.
- 6. If any detail in DATA is unclear or contradictory, respond with "I don't know."

Remember: Every entity in DATA should appear in your final KG. If it's a parameter value (e.g., "Operating Temperature: 80°C"), you can create a Parameter instance. If it's a property (e.g. "Crystallite size: 3.3 nm"), create a Property instance. For materials, manufacturing steps, or measurements, create their corresponding EMMO class instances.

You can store numeric values either as a literal on the node or create a separate node—your choice. But be sure each piece of data is represented as an instance or as a triple-literal if it's a single number.

# **USER INSTRUCTIONS (EMMO Ontology)**

Use only these EMMO classes and object properties:

```
@prefix : <http://emmo.info/emmo#> .
@prefix owl: <http://www.w3.org/2002/07/owl#>
@prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#> .
@prefix xsd: <http://www.w3.org/2001/XMLSchema#>
@prefix rdfs: <http://www.w3.org/2000/01/rdf-schema#> .
@prefix skos: <http://www.w3.org/2004/02/skos/core#> .
:EMMO_4207e895_8b83_4318_996a_72cfb32acd94 rdf:type owl:Class ;
    skos:prefLabel "Material".
:EMMO_a4d66059_5dd3_4b90_b4cb_10960559441b rdf:type owl:Class ;
    skos:prefLabel "Manufacturing".
:EMMO_463bcfda_867b_41d9_a967_211d4d437cfb rdf:type owl:Class ;
    skos:prefLabel "Measurement".
:EMMO_b7bcff25_ffc3_474e_9ab5_01b1664bd4ba rdf:type owl:Class ;
    skos:prefLabel "Property".
:EMMO_dld436e7_72fc_49cd_863b_7bfb4ba5276a rdf:type owl:Class ;
   skos:prefLabel "Parameter".
:EMMO_e1097637 rdf:type owl:ObjectProperty;
   rdfs:domain :EMMO_4207e895_8b83_4318_996a_72cfb32acd94 ;
    rdfs:range :EMMO a4d66059 5dd3 4b90 b4cb 10960559441b ;
   skos:prefLabel "is_manufacturing_input".
:EMMO_e1245987 rdf:type owl:ObjectProperty;
    rdfs:domain :EMMO_a4d66059_5dd3_4b90_b4cb_10960559441b ;
    rdfs:range :EMMO_4207e895_8b83_4318_996a_72cfb32acd94 ;
    skos:prefLabel "has_manufacturing_output".
:EMMO_m5677989 rdf:type owl:ObjectProperty;
    rdfs:domain :EMMO_4207e895_8b83_4318_996a_72cfb32acd94 ;
    rdfs:range :EMMO_463bcfda_867b_41d9_a967_211d4d437cfb ;
    skos:prefLabel "is_measurement_input".
:EMMO m87987545 rdf:type owl:ObjectProperty :
    rdfs:domain :EMMO_463bcfda_867b_41d9_a967_211d4d437cfb ;
    rdfs:range :EMMO_b7bcff25_ffc3_474e_9ab5_01b1664bd4ba ;
    skos:prefLabel "has_measurement_output".
:EMMO_p5778r78 rdf:type owl:ObjectProperty ;
    rdfs:domain :EMMO_4207e895_8b83_4318_996a_72cfb32acd94 ;
```

localhost:8501 4/10 12/30/24, 7:40 PM

```
rdfs:range :EMMO_b7bcff25_ffc3_474e_9ab5_01b1664bd4ba ;
    skos:prefLabel "has_property".

:EMMO_p46903ar7 rdf:type owl:0bjectProperty ;
    rdfs:domain :EMMO_a4d66059_5dd3_4b90_b4cb_10960559441b ;
    rdfs:range :EMMO_d1d436e7_72fc_49cd_863b_7bfb4ba5276a ;
    skos:prefLabel "has_parameter".
```

# **IMPORTANT REMINDER**

- Create instances named ex: Something for every piece of data.
- Combine or link them with the correct object properties.
- Return only the final JSON-LD.
- If uncertain, say "I don't know."

\_\_\_\_\_

DATA: [Insert your real extracted data here, e.g. "Aquivion® PFSA polymer, MEA manufacturing, Operating temperature 80°C," etc. *All these items must appear in the final KG.*] END DATA

=========== DATA (START

Entities: To condense the provided information into a cohesive knowledge graph structure, we can organize the details under distinct categories, identifying key entities and their relationships. Here is how it can be structured:

## Material

- Ionomers and Polymers:
  - o Aquivion® PFSA Polymer
  - o Nafion®
  - o SSC Polymer
- · Catalysts and Alloys:
  - Platinum (Pt)
  - o Platinum-Cobalt (PtCo)
  - 50% Pt on Ketjenblack (Pt/KB)
  - o 50% PtCo on Ketjenblack (PtCo/KB)
- Membranes and Composite Materials:
  - Aquivion®-reinforced membrane R79-01SX+
  - Aguivion® PFSA D79-25BS and D79-20BS
- Other Materials:
  - Ethanol
  - Water (H2O)
  - Cobalt nitrate
  - o Ammonium carbonate
  - Ketjenblack EC

# Manufacturing

- Preparation Processes:
  - $\circ \quad \, \mathsf{MEA} \ (\mathsf{Membrane} \ \mathsf{Electrode} \ \mathsf{Assembly}) \ \mathsf{preparation}$
  - o Electrode preparation
  - Catalytic ink preparation
  - Hot pressing
- Methods:
  - o Deposition

localhost:8501 5/10

## Measurement

- Characterization Techniques:
  - Electrochemical studies and characterization
  - o Transmission Electron Microscopy (TEM)
  - X-ray diffraction (XRD)
  - Scanning Electron Microscopy (SEM)
- Analyses:
  - o Electrochemical Surface Area (ECSA)
  - Steady-state galvanostatic measurements
  - Cyclic voltammetry (CV)

# **Property**

- Ionomer Properties:
  - o Protonic conductivity: High
  - o Chemical stability: High
  - o Thermal stability: High
- Comparison with Nafion®:
  - o Crystallinity, Tg: Higher
  - Swelling: Lower
- Physical Characteristics:
  - o Membrane thickness: 10 μm
  - Equivalent weight of ionomer: 790 g/mol
- Crystallite and Particle Sizes:
  - o Pt in Pt/KB: Crystallite: 2.5 nm, Particle: 2.8 nm
  - o PtCo in PtCo/KB: Crystallite: 3.3 nm, Particle: 3.4 nm

# **Parameter**

- Operating Conditions:
  - o Temperature: 80-95°C
  - o Pressure: 1.5-2 bar abs
  - o Humidity: 50% RH
- Hot Pressing Conditions:
  - Temperature: 125 °C
  - o Pressure: 20 kg/cm<sup>2</sup>
  - Time: 5 min
- Measurement Conditions:
  - Potential range: 20 to 1250 mV
  - Sweep rate: 50 mV/s

This organization illustrates relationships and dependencies among entities in the context, representing a structured approach to constructing a knowledge graph in materials science related to fuel cell technology. Relationships: Based on the extracted relationships from the provided data, the consolidated output is as follows:

## • Manufacturing Inputs:

Critical materials and components like PSFA membrane, PGM catalysts, Aquivion®, Nafion®, catalytic ink, Gas Diffusion Layer Sigracet-25BC, electrodes, R79-01SX+ membrane, catalyst powder, CU grid, 2-propanol, Pt, and PtCo are identified as essential inputs in the manufacturing process of fuel cell components.

## Manufacturing Outputs:

 The process yields products such as membrane-electrode assemblies (MEAs), Pt/KB, and PtCo/KB.

localhost:8501 6/10

12/30/24, 7:40 PM

#### Measurement Inputs:

• Electrocatalyst powders, Pt/KB, PtCo/KB, and MEA are utilized in performance measurements.

mini5

## • Measurement Outputs:

 Results include detailed analysis such as morphology, crystallographic structure, degree of alloying, crystallite sizes, polarization curves, mass activity (j m), and electro-kinetic parameters (ECSA, jm @ 0.9V IRfree).

## · Properties:

 Various characteristics such as catalyst powder, Pt loading, crystallite sizes, and commercial gas diffusion layer (Sigracet-25BC) are noted, alongside electrochemical surface area (ECSA), MEArelated parameters (ECSA, jm @ 0.9V IRfree).

## • Parameters:

• Includes morphology, crystallographic structure, degree of alloying, potential, and sweep rate, which are critical for assessing and optimizing fuel cell performance.

To apply this information effectively in a materials ontology framework like EMMO, detailed information about each category from academic sources would be necessary, focusing on materials, manufacturing processes, measurements, and properties to draw specific conclusions and relationships. DATA (END)

Download JSON Generation Agent Output

#### Generated JSON-LD:

```
G
"@context": {
 "ex": "http://example.com/",
 "emmo": "http://emmo.info/emmo#"
},
"@graph": [
    "@id": "ex:Aquivion_PFSA_Polymer",
    "@type": "emmo:EMMO_4207e895_8b83_4318_996a_72cfb32acd94"
 },
    "@id": "ex:Nafion",
    "@type": "emmo:EMMO_4207e895_8b83_4318_996a_72cfb32acd94"
    "@id": "ex:SSC_Polymer",
    "@type": "emmo:EMMO_4207e895_8b83_4318_996a_72cfb32acd94"
    "@id": "ex:Platinum",
    "@type": "emmo:EMMO_4207e895_8b83_4318_996a_72cfb32acd94"
 },
    "@id": "ex:Platinum_Cobalt",
    "@type": "emmo:EMMO_4207e895_8b83_4318_996a_72cfb32acd94"
 },
    "@id": "ex:50_Pt_on_Ketjenblack",
    "@type": "emmo:EMMO_4207e895_8b83_4318_996a_72cfb32acd94"
    "@id": "ex:50_PtCo_on_Ketjenblack",
    "@type": "emmo:EMMO_4207e895_8b83_4318_996a_72cfb32acd94"
 },
    "@id": "ex:Aquivion_reinforced_membrane_R79_01SX",
    "@type": "emmo:EMMO_4207e895_8b83_4318_996a_72cfb32acd94"
    "@id": "ex:Aquivion_PFSA_D79_25BS",
```

localhost:8501 7/10

```
"@type": "emmo:EMMO_4207e895_8b83_4318_996a_72cfb32acd94"
},
  "@id": "ex:Aquivion_PFSA_D79_20BS",
  "@type": "emmo:EMMO_4207e895_8b83_4318_996a_72cfb32acd94"
},
  "@id": "ex:Ethanol",
  "@type": "emmo:EMMO_4207e895_8b83_4318_996a_72cfb32acd94"
},
  "@id": "ex:Water",
  "@type": "emmo:EMMO_4207e895_8b83_4318_996a_72cfb32acd94"
}.
  "@id": "ex:Cobalt_nitrate",
  "@type": "emmo:EMMO_4207e895_8b83_4318_996a_72cfb32acd94"
},
  "@id": "ex:Ammonium_carbonate",
  "@type": "emmo:EMMO_4207e895_8b83_4318_996a_72cfb32acd94"
  "@id": "ex:Ketjenblack_EC",
  "@type": "emmo:EMMO_4207e895_8b83_4318_996a_72cfb32acd94"
},
  "@id": "ex:MEA_preparation",
  "@type": "emmo:EMMO_a4d66059_5dd3_4b90_b4cb_10960559441b"
},
  "@id": "ex:Electrode_preparation",
  "@type": "emmo:EMMO_a4d66059_5dd3_4b90_b4cb_10960559441b"
},
  "@id": "ex:Catalytic_ink_preparation",
  "@type": "emmo:EMMO_a4d66059_5dd3_4b90_b4cb_10960559441b"
},
  "@id": "ex:Hot_pressing",
  "@type": "emmo:EMMO_a4d66059_5dd3_4b90_b4cb_10960559441b"
},
  "@id": "ex:Deposition",
  "@type": "emmo:EMMO_a4d66059_5dd3_4b90_b4cb_10960559441b"
},
  "@id": "ex:Electrochemical_studies_and_characterization",
  "@type": "emmo:EMMO_463bcfda_867b_41d9_a967_211d4d437cfb"
  "@id": "ex:Transmission_Electron_Microscopy",
  "@type": "emmo:EMMO_463bcfda_867b_41d9_a967_211d4d437cfb"
},
  "@id": "ex:X_ray_diffraction",
  "@type": "emmo:EMMO_463bcfda_867b_41d9_a967_211d4d437cfb"
},
  "@id": "ex:Scanning_Electron_Microscopy",
  "@type": "emmo:EMMO_463bcfda_867b_41d9_a967_211d4d437cfb"
},
  "@id": "ex:Electrochemical_Surface_Area",
  "@type": "emmo:EMMO_463bcfda_867b_41d9_a967_211d4d437cfb"
},
  "@id": "ex:Steady_state_galvanostatic_measurements",
```

```
"@type": "emmo:EMMO_463bcfda_867b_41d9_a967_211d4d437cfb"
},
  "@id": "ex:Cyclic_voltammetry",
  "@type": "emmo:EMMO_463bcfda_867b_41d9_a967_211d4d437cfb"
},
  "@id": "ex:Protonic_conductivity",
  "@type": "emmo:EMMO_b7bcff25_ffc3_474e_9ab5_01b1664bd4ba",
  "value": "High"
},
  "@id": "ex:Chemical_stability",
  "@type": "emmo:EMMO_b7bcff25_ffc3_474e_9ab5_01b1664bd4ba",
  "value": "High"
},
  "@id": "ex:Thermal_stability",
  "@type": "emmo:EMMO_b7bcff25_ffc3_474e_9ab5_01b1664bd4ba",
  "value": "High"
  "@id": "ex:Crystallinity",
  "@type": "emmo:EMMO_b7bcff25_ffc3_474e_9ab5_01b1664bd4ba",
  "property_of": "ex:Nafion",
  "comparison": "Higher"
},
  "@id": "ex:Tg",
  "@type": "emmo:EMMO_b7bcff25_ffc3_474e_9ab5_01b1664bd4ba",
  "property_of": "ex:Nafion",
  "comparison": "Higher"
  "@id": "ex:Swelling",
 "@type": "emmo:EMMO_b7bcff25_ffc3_474e_9ab5_01b1664bd4ba",
  "property_of": "ex:Nafion",
  "comparison": "Lower"
},
  "@id": "ex:Membrane_thickness",
  "@type": "emmo:EMMO_b7bcff25_ffc3_474e_9ab5_01b1664bd4ba",
  "value": "10 μm"
},
  "@id": "ex:Equivalent_weight_of_ionomer",
  "@type": "emmo:EMMO_b7bcff25_ffc3_474e_9ab5_01b1664bd4ba",
  "value": "790 g/mol"
},
  "@id": "ex:Crystallite_size_Pt",
  "@type": "emmo:EMMO_b7bcff25_ffc3_474e_9ab5_01b1664bd4ba",
  "property_of": "ex:50_Pt_on_Ketjenblack",
  "value": "2.5 nm"
},
  "@id": "ex:Particle_size_Pt",
  "@type": "emmo:EMMO_b7bcff25_ffc3_474e_9ab5_01b1664bd4ba",
  "property_of": "ex:50_Pt_on_Ketjenblack",
  "value": "2.8 nm"
},
  "@id": "ex:Crystallite_size_PtCo",
  "@type": "emmo:EMMO_b7bcff25_ffc3_474e_9ab5_01b1664bd4ba",
  "property_of": "ex:50_PtCo_on_Ketjenblack",
  "value": "3.3 nm"
},
```

```
"@id": "ex:Particle_size_PtCo",
  "@type": "emmo:EMMO_b7bcff25_ffc3_474e_9ab5_01b1664bd4ba",
  "property_of": "ex:50_PtCo_on_Ketjenblack",
  "value": "3.4 nm"
},
  "@id": "ex:Operating_Temperature",
 "@type": "emmo:EMMO_d1d436e7_72fc_49cd_863b_7bfb4ba5276a",
  "value": "80-95°C"
},
  "@id": "ex:Operating_Pressure",
  "@type": "emmo:EMMO_dld436e7_72fc_49cd_863b_7bfb4ba5276a",
  "value": "1.5-2 bar abs"
},
  "@id": "ex:Humidity",
  "@type": "emmo:EMMO_d1d436e7_72fc_49cd_863b_7bfb4ba5276a",
  "value": "50% RH"
},
  "@id": "ex:Hot_Pressing_Temperature",
  "@type": "emmo:EMMO_d1d436e7_72fc_49cd_863b_7bfb4ba5276a",
  "value": "125 °C"
  "@id": "ex:Hot_Pressing_Pressure",
  "@type": "emmo:EMMO_d1d436e7_72fc_49cd_863b_7bfb4ba5276a",
  "value": "20 kg/cm<sup>2</sup>"
},
  "@id": "ex:Hot_Pressing_Time",
 "@type": "emmo:EMMO_d1d436e7_72fc_49cd_863b_7bfb4ba5276a",
 "value": "5 min"
  "@id": "ex:Measurement_Potential_range",
 "@type": "emmo:EMMO_d1d436e7_72fc_49cd_863b_7bfb4ba5276a",
  "value": "20 to 1250 mV"
},
  "@id": "ex:Sweep_rate",
 "@type": "emmo:EMMO_d1d436e7_72fc_49cd_863b_7bfb4ba5276a",
  "value": "50 mV/s"
```

Validation failed: Expecting value: line 1 column 1 (char 0)

localhost:8501 10/10