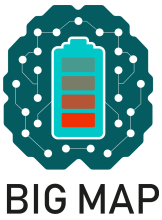
# Battery INterFace Ontology (BattINFO) Reference Documentation

Version 0.0.1

Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)

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**Abstract**

This is a reference documentation for the Battery Interface Ontology (BattINFO).

BattINFO is an ontology of batteries and their interfaces based on the top-level European Materials and Modelling Ontology (EMMO). BattINFO aims to formalize the current state of knowledge on battery interfaces to support the development of computational tools and the deployment of interoperable data in the BIG-MAP project and beyond. The definitions included in BattINFO are based as far as possible on accepted standards defined by the International Union of Pure and Applied Chemistry (IUPAC) or other preeminent textbooks on the subject. BattINFO objects and their relations to each other are designed with three goals in mind: (i) to be scientifically rigorous and accurate, (ii) to reflect current battery orthodoxy and dominant jargon, and (iii) to be flexible to describe a range of battery chemistries, not only Li-ion.

The development of BattINFO is a mammoth undertaking and will continue throughout the project. However, it is important to establish an initial version to support the activities in other BIG-MAP work packages and provide a preliminary platform for collaboration. The objective of this deliverable is to establish the initial version of BattINFO. This report outlines the conceptual foundation for the definitions in the ontology and serves as a guide to help interpret the implementation of BattINFO in the ontology web language (OWL).

**Keywords:** Battery, EMMO, materials science, modelling, characterisation, materials, ontology

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# Contents

# Chapter 1

# Introduction

Battery development is one of the most important and intensely pursued technical research topics in the world today. From personal electronics to electric mobility to renewable energy storage, batteries are essential to progress. The search for better batteries is supported by a host of databases, methods, models, publications, and presentations. How can we distil this deluge of data into knowledge and translate that knowledge into action?

The answer must rely in some part on artificial intelligence (AI). The breadth of fields necessary to completely describe of battery performance, characterization, and simulation combined with the depth of research being generated in those fields is simply too great for any single person (or even group of people) to manage. However, the challenge is that the wealth of battery data that exists is formatted to be read, understood, and learned by humans, not machines. The field needs a tool to formalize the current state of knowledge about battery interfaces that is both human- and machine-readable.

The Battery Interface Ontology (BattINFO) is a domain ontology for batteries and their interfaces. It is developed with the goal of creating a formalized description of battery cells to support the interoperability of battery data and support applications of artificial intelligence in battery research.

BattINFO builds upon long-standing and widely accepted principles of electrochemistry as described in preeminent texts such as Electrochemical Systems by John Newman and Karen E. Thomas-Alyea [1], Electrochemical Methods: Fundamentals and Applications by Allen J. Bard and Larry R. Faulkner [2], and Handbook of Batteries by David Linden and Thomas B. Reddy [3], among other seminal sources [4], [5]. The terminology adheres as far as possible to the recommendations and definitions contained in the Compendium of Chemical Terminology (also known as the "Gold Book") from the International Union of Pure and Applied Chemistry (IUPAC) [6] together with IUPAC supplements on electrochemical terminology [7] and recommendations from the Electrochemical Society (ECS) on nomenclature and standards. Places where conflicts exist between sources are noted for further discussion and resolution within the electrochemical community.

BattINFO employs the European Materials and Modelling Ontology (EMMO) as a top-level ontology. EMMO aims at the development of a standard representational ontology framework based on current materials modelling and characterization of knowledge. EMMO starts from the very basic scientific fundamentals and grows to encompass a complex and wide field of knowledge, however it is still functional and clear. This makes it ideal to support the development of BattINFO as an EMMO domain ontology.

The purpose of this report is to lay the groundwork for the development of BattINFO in the BIG-MAP project.

## Availability and license

The Battery Interface Domain Ontology is available from the github repository https://github.com/BIG-MAP/BattINFO.

# References


1. J. Newman and K. E. Thmoas-Alyea, Electrochemical Systems, 3rd ed. Hoboken, New Jersey: John Wiley & Sons, 2004.
2. A. J. Bard and L. R. Faulkner, ELECTROCHEMICAL METHODS: Fundamentals and applications. 2001.
3. D. Linden and T. Reddy, Handbook of Batteries. 2002.
4. P. Atkins and J. De Paula, Atkins' Physical Chemistry, 8th Ed. New York: W.H. Freeman and Company, 2006.
5. M. Pourbaix, Atlas of Electrochemical Equilibria in Aqueous Solutions, Second. Houston, Texas: National Association of Corrosion Engineers, 1974.
6. IUPAC, Compendium of Chemical Terminology, 2nd (the ". Oxford: Blackwell Scientific Publications, 2014.
7. J. M. Pingarrón et al., Terminology of electrochemical methods of analysis (IUPAC Recommendations 2019), Pure Appl. Chem., vol. 92, no. 4, pp. 641-694, 2020.

# Chapter 2

# Generic concepts

These classes are intended to be merged back into EMMO.

## Participant subclasses

### ActiveParticipant

**IRI:** http://emmo.info/emmo#EMMO_038e37a3_1684_4980_b5e4_67ab34cd5bdb

**Elucidation:** A 'physical' that stands for a real world object that takes active part of a functional process.

**Preflabel:** ActiveParticipant

**Relations:**

- is_a emmo.Participant
- Inverse(emmo.hasProperParticipant) some emmo.FunctionalProcess

### FunctionalMaterial

**IRI:** http://emmo.info/emmo#EMMO_d95e6e0d-e8eb-411a-b407-0d1a517e8767

**Elucidation:** Materials that have one or more properties that can be significantly changed in a controlled fashion by external stimuli (temperature, electric/magnetic field, etc.) and are therefore applied in a broad range of technological devices as for example in memories, displays and telecommunication. - NTNU FY3114 - Functional Materials

**Preflabel:** FunctionalMaterial

**Relations:**

- is_a emmo.ActiveParticipant
- is_a emmo.Material

## Process subclasses

### FunctionalProcess

**IRI:** http://emmo.info/emmo#EMMO_f7dbce66_2822_4855_9f42_1da71aa9e923

**Elucidation:** The process that makes a product work as intended when in use.

**Example:** - The light-emitting process of a diode. - The car crash process for a crash box in a car. - The discharging process of a battery.

**Preflabel:** FunctionalProcess

**Relations:**

- is_a emmo.Process

### ChemicalPhenomenon

**IRI:** http://emmo.info/emmo#EMMO_50e36d79_b2dd_422d_81eb_a665028a1ead

**Elucidation:** A 'process' that is recognized by chemical sciences and is catogrized accordingly.

**Preflabel:** ChemicalPhenomenon

**Relations:**

- is_a emmo.Process

### ChemicalReaction

**IRI:** http://emmo.info/emmo#EMMO_ecb0395f_ee1e_4e9a_bf5c_d8e56eee2d18

**Elucidation:** A process that results in the interconversion of chemical species. Chemical reactions may be elementary reactions or stepwise reactions. (It should be noted that this definition includes experimentally observable interconversions of conformers.) Detectable chemical reactions normally involve sets of molecular entities as indicated by this definition, but it is often conceptually convenient to use the term also for changes involving single molecular entities (i.e. 'microscopic chemical events').

- IUPAC Gold Book

**Preflabel:** ChemicalReaction

**Relations:**

- is_a emmo.ChemicalPhenomenon

## Physicalistic subclasses

### Pore

**IRI:** http://emmo.info/emmo#EMMO_69b9aead-bb43-4bd5-9168-728cea2116b1

**Elucidation:** A space within a solid host domain that is filled by a liquid, gas, or vacuum. The characteristic length of the pore is much less than the characteristic length of the host domain. An exception is possible for 1 dimension (e.g. long pores).

**Preflabel:** Pore

**Relations:**

- is_a emmo.Physicalistic
- emmo.hasContactWith some emmo.Solid
- is_a emmo.Gas or emmo.Vacuum or emmo.Liquid

## Physical quantities

### VolumetricThermalExpansionCoefficient

**IRI:** http://emmo.info/emmo#EMMO_1c1ec02e_4def_4979_aff9_572c06a95391

**Physicaldimension:** T0 L0 M0 I0 Θ-1 N0 J0

**Preflabel:** VolumetricThermalExpansionCoefficient

**Relations:**

- is_a emmo.ThermalExpansionCoefficient

### SingleComponentDiffusivity

**IRI:** http://emmo.info/emmo#EMMO_498d80ae_9339_49c7_8c74_44aa704e0395

**Elucidation:** Transport of particles belonging to one component of a material due to a concentration gradient.

**Physicaldimension:** T-1 L+2 M0 I0 Θ0 N-1 J0

**Preflabel:** SingleComponentDiffusivity

**Relations:**

- is_a emmo.PhysicoChemical
- is_a emmo.ISQDerivedQuantity

### SingleComponentDiffusivity

**IRI:** http://emmo.info/emmo#EMMO_498d80ae_9339_49c7_8c74_44aa704e0395

**Elucidation:** Transport of particles belonging to one component of a material due to a concentration gradient.

**Physicaldimension:** T-1 L+2 M0 I0 Θ0 N-1 J0

**Preflabel:** SingleComponentDiffusivity

**Relations:**

- is_a emmo.PhysicoChemical
- is_a emmo.ISQDerivedQuantity

### SingleComponentMaximalDiffusivity

**IRI:** http://emmo.info/emmo#EMMO_3bd39834_7eb9_4c97_bb25_db88c3df6bab

**Etymology:** Pre-factor in the Arrhenius expression for diffusion.

**Physicaldimension:** T-1 L+2 M0 I0 Θ0 N-1 J0

**Preflabel:** SingleComponentMaximalDiffusivity

**Relations:**

- is_a emmo.ISQDerivedQuantity
- is_a emmo.PhysicoChemical

### SingleComponentActivationEnergyOfDiffusion

**IRI:** http://emmo.info/emmo#EMMO_2f761aff_88d1_4e79_a85e_09d6f400de56

**Elucidation:** The energy barrier for diffusion of a given component.

**Physicaldimension:** T-2 L+2 M+1 I0 Θ0 N0 J0

**Preflabel:** SingleComponentActivationEnergyOfDiffusion

**Relations:**

- is_a emmo.PhysicoChemical
- is_a emmo.Energy

## MolarHeatCapacity

**IRI:** http://emmo.info/emmo#EMMO_50c5d440_683c_400f_909e_b03c0327de9c

**Elucidation:** The molar heat capacity of a substance is the heat capacity of one mole of material.

**Physicaldimension:** T-2 L+2 M+1 I0 Θ-1 N-1 J0

**Preflabel:** MolarHeatCapacity

**Relations:**

- is_a emmo.ISQDerivedQuantity
- is_a emmo.PhysicoChemical

## EnergyDensity

**IRI:** http://emmo.info/emmo#EMMO_686308bd_8ed6_49d0_a204_6487dbe56511

**Elucidation:** Energy per unit volume.

**Physicaldimension:** T-2 L+2 M+1 I0 Θ0 N0 J0

**Preflabel:** EnergyDensity

**Relations:**

- is_a emmo.ISQDerivedQuantity

## ThermalExpansionCoefficient

**IRI:** http://emmo.info/emmo#EMMO_7684ddff_d99b_405d_aad2_90e830b8403c

**Elucidation:** The coefficient of thermal expansion describes how the fractional change in size of an object changes with a change in temperature.

**Physicaldimension:** T0 L0 M0 I0 Θ-1 N0 J0

**Preflabel:** ThermalExpansionCoefficient

**Relations:**

- is_a emmo.ISQDerivedQuantity
- is_a emmo.PhysicoChemical

## HeatCapacity

**IRI:** http://emmo.info/emmo#EMMO_802c167d_b792_4cb8_a315_35797345c0e3

**Elucidation:** The amount of heat to be applied to a given mass of material to produce a unit change in its temperature.

**Physicaldimension:** T-2 L+2 M+1 I0 Θ-1 N0 J0

**Preflabel:** HeatCapacity

**Relations:**

- is_a emmo.ISQDerivedQuantity
- is_a emmo.PhysicoChemical

### ThermalConductivity

**IRI:** http://emmo.info/emmo#EMMO_8dd40ec6_2c5a_43f3_bf64_cadcd447a1c1

**Elucidation:** The ability of a material to conduct heat.

**Physicaldimension:** T-3 L+1 M+1 I0 Θ-1 N0 J0

**Preflabel:** ThermalConductivity

**Relations:**

- is_a emmo.ISQDerivedQuantity
- is_a emmo.PhysicoChemical

### SpecificHeatCapacity

**IRI:** http://emmo.info/emmo#EMMO_b4f4ed28_d24c_4a00_9583_62ab839abeca

**Elucidation:** The specific heat capacity (symbol cp) of a substance is the heat capacity of a sample of the substance divided by the mass of the sample.

**Physicaldimension:** T-2 L+2 M0 I0 Θ-1 N0 J0

**Preflabel:** SpecificHeatCapacity

**Relations:**

- is_a emmo.ISQDerivedQuantity
- is_a emmo.PhysicoChemical

## Additional quantity dimensions

### PerTemperatureDimension

**IRI:** http://emmo.info/emmo#EMMO_6e9aef15_272b_4eea_aaa9_2f38b8ae951f

**Preflabel:** PerTemperatureDimension

**Relations:**

- is_a emmo.PhysicalDimension
- equivalent_to emmo.hasSymbolData value “T0 L0 M0 I0 Θ-1 N0 J0”

# Chapter 3

# Electrochemical and battery-specific concepts

All classes under here are defined with the http://emmo.info/BattINFO# namespace.

## Active Participant branch

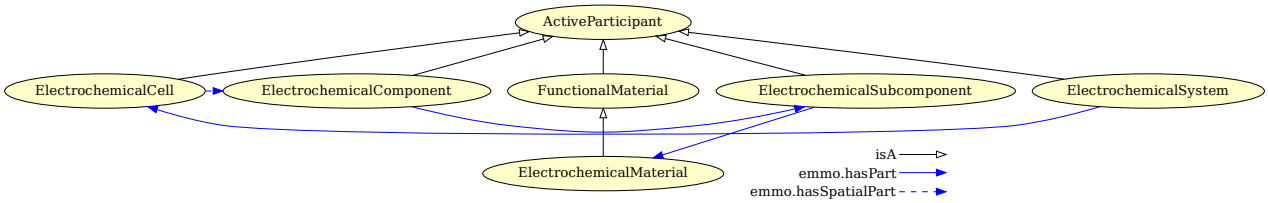


Figure 3.1: Active Participant branch.

### FunctionalMaterial

**IRI:** http://emmo.info/emmo#EMMO_d95e6e0d-e8eb-411a-b407-0d1a517e8767

**Elucidation:** Materials that have one or more properties that can be significantly changed in a controlled fashion by external stimuli (temperature, electric/magnetic field, etc.) and are therefore applied in a broad range of technological devices as for example in memories, displays and telecommunication. - NTNU FY3114 - Functional Materials

**Preflabel:** FunctionalMaterial

**Relations:**

- is_a emmo.ActiveParticipant
- is_a emmo.Material

### ActiveParticipant

**IRI:** http://emmo.info/emmo#EMMO_038e37a3_1684_4980_b5e4_67ab34cd5bdb

**Elucidation:** A 'physical' that stands for a real world object that takes active part of a functional process.

**Preflabel:** ActiveParticipant

**Relations:**

- is_a emmo.Participant
- Inverse(emmo.hasProperParticipant) some emmo.FunctionalProcess

# Electrochemical System branch

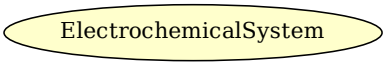


Figure 3.2: Electrochemical System branch.

## ElectrochemicalSystem

**IRI:** http://emmo.info/BattINFO#EMMO_4e4d7f4b-680b-469e-bdd4-728dd3e465bf

**Elucidation:** A system comprising at least one electrochemical cell and the components necessary to support it.

**Preflabel:** ElectrochemicalSystem

**Relations:**

- is_a emmo.ActiveParticipant
- emmo.hasPart some BattINFO.ElectrochemicalCell

# Electrochemical Cell branch

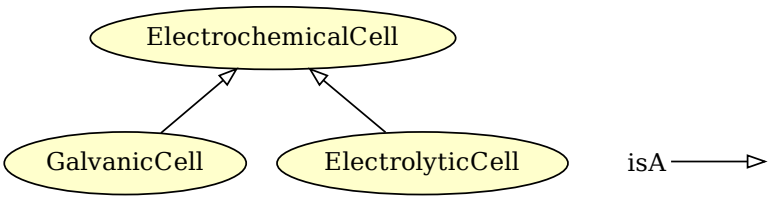


Figure 3.3: Electrochemical Cell branch.

## GalvanicCell

**IRI:** http://emmo.info/BattINFO#EMMO_e248373f_294f_4ca4_9edf_0ad6653bb64f

**Elucidation:** An electrochemical cell that spontaneously produces work.

– J. Newman, Electrochemical Systems (p. 6)

**Preflabel:** GalvanicCell

**Relations:**

- is_a BattINFO.ElectrochemicalCell

### ElectrochemicalCell

**IRI:** http://emmo.info/BattINFO#EMMO_6f2c88c9_5c04_4953_a298_032cc3ab9b77

**Elucidation:** A system capable of either generating electrical energy from chemical reactions or using electrical energy to cause chemical reactions. The key feature of an electrochemical cell is that it contains two (or more) electrodes that allow transport of electrons, separated by a salt bridge that allows the movement of ions but blocks movement of electrons.

– Adapted from J. Newman, Electrochemical Systems (p. 3) and other sources

**Preflabel:** ElectrochemicalCell

**Relations:**

- is_a emmo.Matter
- is_a emmo.Object
- is_a emmo.ActiveParticipant
- emmo.hasConventionalQuantity some emmo.HeatCapacity
- emmo.hasSpatialPart some BattINFO.ElectrochemicalComponent
- emmo.hasConventionalQuantity some emmo.ThermalConductivity
- emmo.hasConventionalQuantity some emmo.Mass
- emmo.hasConventionalQuantity some emmo.ElectricPotential
- emmo.hasConventionalQuantity some BattINFO.ChargeCapacity
- emmo.hasConventionalQuantity some emmo.ThermodynamicTemperature
- emmo.hasConventionalQuantity some BattINFO.StoredEnergy
- emmo.hasConventionalQuantity some BattINFO.InternalConductance
- emmo.hasConventionalQuantity some BattINFO.InternalResistance
- emmo.hasConventionalQuantity some emmo.ThermalExpansionCoefficient
- emmo.hasConventionalQuantity some BattINFO.SpecificEnergy
- emmo.hasConventionalQuantity some emmo.SpecificHeatCapacity
- emmo.hasConventionalQuantity some emmo.Volume
- emmo.hasConventionalQuantity some BattINFO.SpecificChargeCapacity
- emmo.hasConventionalQuantity some BattINFO.OpenCircuitVoltage
- emmo.hasConventionalQuantity some emmo.EnergyDensity
- emmo.hasConventionalQuantity some emmo.Density
- emmo.hasConventionalQuantity some emmo.ElectricImpedance

### ElectrolyticCell

**IRI:** http://emmo.info/BattINFO#EMMO_e931087f_7681_4096_b200_5223bcc47eb4

**Elucidation:** An electrochemical cell that requires input of work to drive the reaction.

– J. Newman, Electrochemical Systems (p. 6)

**Preflabel:** ElectrolyticCell

**Relations:**

- is_a BattINFO.ElectrochemicalCell

## Electrochemical Component branch

### Separator

**IRI:** http://emmo.info/BattINFO#EMMO_331e6cca_f260_4bf8_af55_35304fe1bbe0

**Definition:** "A permeable membrane placed between the positive and negative electrodes to keep them physically separated and prevent an internal short circuit."

**Preflabel:** Separator

**Relations:**

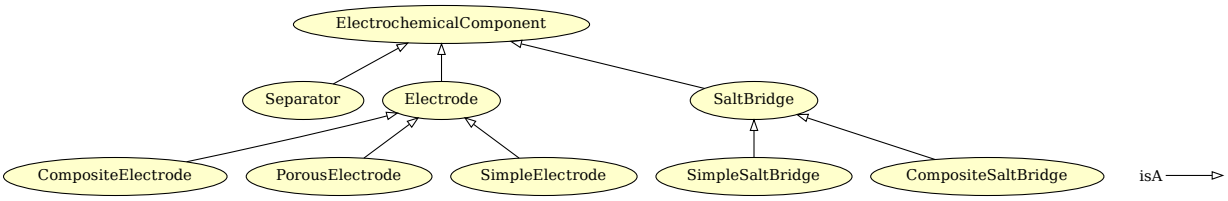


Figure 3.4: Electrochemical Component branch.

- is_a BattINFO.ElectrochemicalComponent

## CompositeElectrode

**IRI:** http://emmo.info/BattINFO#EMMO_7aa79b12-6b34-4724-9728-f31b5f7ed83d

**Elucidation:** An electrode consisting of multiple ElectrochemicalSubComponent

**Preflabel:** CompositeElectrode

**Relations:**

- is_a BattINFO.Electrode

## PorousElectrode

**IRI:** http://emmo.info/BattINFO#EMMO_3663991d-9319-4f7a-922b-f0e428b58801

**Elucidation:** Porous electrodes consist of porous matrices of a single reactive electronic conductor or a mixture of solids that include essentially non-conducting, reactive materials in addition to electronic conductors. An electrolytic solution fills the void spaces of the porous matrix. At a given time, there may be a large range of reaction rates within the pores. The distribution of these rates will depend on physical structure, conductivity of the matrix and of the electrolyte, and on parameters characterizing the electrode processes themselves. - Newman and Thomas-Alyea, Electrochemical Systems.

**Preflabel:** PorousElectrode

**Relations:**

- is_a BattINFO.Electrode
- emmo.hasSpatialPart some BattINFO.ElectrodePore

## ElectrochemicalComponent

**IRI:** http://emmo.info/BattINFO#EMMO_3597a1e0_09ef_48ad_b913_b3e71ea21c94

**Elucidation:** A component that is essential to the function of an electrochemical cell.

**Preflabel:** ElectrochemicalComponent

**Relations:**

- is_a emmo.ActiveParticipant
- emmo.hasPart some BattINFO.ElectrochemicalSubcomponent

## SimpleSaltBridge

**IRI:** http://emmo.info/BattINFO#EMMO_6e4f4681-f327-4300-96e4-5905fcea36e3

**Elucidation:** A salt bridge consisting of exactly 1 subcomponent that is an IonicSubcomponent.

**Preflabel:** SimpleSaltBridge

**Relations:**

- is_a BattINFO.SaltBridge
- is_a emmo.State
- emmo.hasSpatialDirectPart exactly 1 BattINFO.IonicSubcomponent

## CompositeSaltBridge

**IRI:** http://emmo.info/BattINFO#EMMO_6cae5943-737a-4f88-9903-9de4cffebd11

**Elucidation:** A salt bridge consisting of at least two subcomponents, one of which is an IonicSubcomponent.

**Preflabel:** CompositeSaltBridge

**Relations:**

- is_a BattINFO.SaltBridge
- is_a emmo.State
- emmo.hasSpatialDirectPart some BattINFO.IonicSubcomponent
- emmo.hasSpatialDirectPart min 2 BattINFO.ElectrochemicalSubcomponent

## Electrode

**IRI:** http://emmo.info/BattINFO#EMMO_0f007072-a8dd-4798-b865-1bf9363be627

**Elucidation:** Electron conductor in an electrochemical cell connected to the external circuit. - Terminology of electrochemical methods of analysis (IUPAC Recommendations 2019)

**Preflabel:** Electrode

**Relations:**

- is_a emmo.Object
- is_a BattINFO.ElectrochemicalComponent
- emmo.hasContactWith some BattINFO.Electrolyte
- emmo.hasConventionalQuantity some BattINFO.ChargeCapacity

## SimpleElectrode

**IRI:** http://emmo.info/BattINFO#EMMO_029f0b45-70a7-481f-8154-bf982a77e08c

**Elucidation:** An electrode consisting of a single ElectrochemicalSubComponent

**Example:** Metal foil.

**Preflabel:** SimpleElectrode

**Relations:**

- is_a BattINFO.Electrode

## SaltBridge

**IRI:** http://emmo.info/BattINFO#EMMO_637c576e_a50e_47ae_8c74_2024ce4c6d0f

**Elucidation:** “Means of making electrolytic connection between two half cells without introducing a significant liquid junction potential. Note: A typical construction is a tube of an inert material (e.g. agar agar) filled with a solution con- taining an electrolyte with approximately equal ion mobilities of the cation and the anion (e.g., KNO3, KCl), with the ends of the tube immersed in the electrolyte solution of the half cells.” Pingarron et al., Terminology of electrochemical methods of analysis

**Preflabel:** SaltBridge

**Relations:**

- is_a BattINFO.ElectrochemicalComponent

# Electrochemical Subcomponent branch

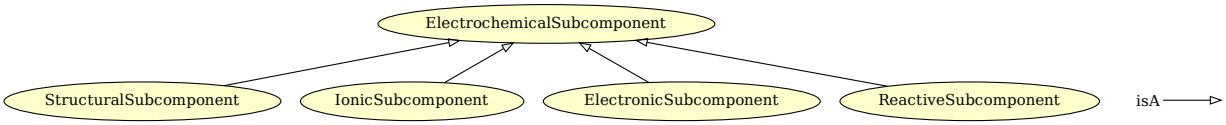


Figure 3.5: Electrochemical Subcomponent branch.

## StructuralSubcomponent

**IRI:** http://emmo.info/BattINFO#EMMO_dd15b4b0-11e7-4900-b379-9702a8caa6bb

**Preflabel:** StructuralSubcomponent

**Relations:**

- is_a BattINFO.ElectrochemicalSubcomponent

## IonicSubcomponent

**IRI:** http://emmo.info/BattINFO#EMMO_23b866e8-27c6-4fd8-a1d2-6b58ad4445af

**Preflabel:** IonicSubcomponent

**Relations:**

- is_a BattINFO.ElectrochemicalSubcomponent

## ElectronicSubcomponent

**IRI:** http://emmo.info/BattINFO#EMMO_9c4e61c6-4a7b-41c2-9133-e780e144ddcd

**Elucidation:** An ElectrochemicalSubcomponent whose primary role is electronic

**Example:** Current Collector Conducting Additive

**Preflabel:** ElectronicSubcomponent

**Relations:**

- is_a BattINFO.ElectrochemicalSubcomponent

## ElectrochemicalSubcomponent

**IRI:** http://emmo.info/BattINFO#EMMO_f89bb8bc-ef9b-43d5-b5df-14e12b0d93b8

**Elucidation:** A subcomponent of an ElectrochemicalComponent.

**Preflabel:** ElectrochemicalSubcomponent

**Relations:**

- is_a emmo.ActiveParticipant
- emmo.hasPart some BattINFO.ElectrochemicalMaterial

### ReactiveSubcomponent

**IRI:** http://emmo.info/BattINFO#EMMO_6ab1ca1a-3809-4e9a-aaf7-374915288f73

**Elucidation:** An ElectrochemicalSubcomponent whose primary role is to participate in a reaction.

**Preflabel:** ReactiveSubcomponent

**Relations:**

- is_a BattINFO.ElectrochemicalSubcomponent

## Electrochemical Material branch

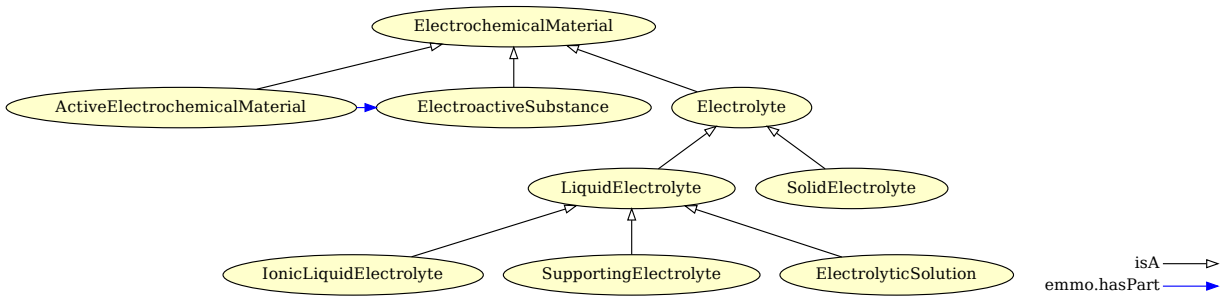


Figure 3.6: Electrochemical Material branch.

### ActiveElectrochemicalMaterial

**IRI:** http://emmo.info/BattINFO#EMMO_79d1b273-58cd-4be6-a250-434817f7c261

**Preflabel:** ActiveElectrochemicalMaterial

**Relations:**

- is_a BattINFO.ElectrochemicalMaterial
- emmo.hasPart some BattINFO.ElectroactiveSubstance

### ElectroactiveSubstance

**IRI:** http://emmo.info/BattINFO#EMMO_92ba4a12-146e-4b1f-86f3-bcc66ac52763

**Preflabel:** ElectroactiveSubstance

**Relations:**

- is_a BattINFO.ElectrochemicalMaterial

### IonicLiquidElectrolyte

**IRI:** http://emmo.info/BattINFO#EMMO_c3f4b34a_0e2c_46f3_baab_4ebd2682d26f

**Definition:** “An ionic liquid is an electrolyte composed of a salt that is liquid below 100 °C. Ionic liquids have found uses in electrochemical analysis, because their unconventional properties include a negligible vapor pressure, a high thermal and electrochemical stability, and exceptional dissolution properties for both organic and inorganic chemical species.” Pingarron et al., Terminology of electrochemical methods of analysis

**Preflabel:** IonicLiquidElectrolyte

**Relations:**

- is_a BattINFO.LiquidElectrolyte

### SupportingElectrolyte

**IRI:** http://emmo.info/BattINFO#EMMO_1fc5642c_b7b2_43bf_ad20_f96001db8800

**Definition:** "Electrolyte solution, the ions of which are electroinactive in the range of applied potential being studied, and whose ionic strength (and, therefore, contribution to the overall conductivity) is usually much greater than the concentration of an electroactive substance to be dissolved in it." Pingarron et al., Terminology of electrochemical methods of analysis

**Preflabel:** SupportingElectrolyte

**Relations:**

- is_a BattINFO.LiquidElectrolyte

### LiquidElectrolyte

**IRI:** http://emmo.info/BattINFO#EMMO_609b340f_3450_4a10_95c2_c457e3eb8a89

**Definition:** "An electrolyte in the liquid phase"

**Preflabel:** LiquidElectrolyte

**Relations:**

- is_a BattINFO.Electrolyte

### Electrolyte

**IRI:** http://emmo.info/BattINFO#EMMO_fb0d9eef_92af_4628_8814_e065ca255d59

**Definition:** 1. Conducting medium in which the flow of electric current is accompanied by the movement of ions. Pingarron et al., Terminology of electrochemical methods of analysis

**Preflabel:** Electrolyte

**Relations:**

- is_a BattINFO.ElectrochemicalMaterial

### ElectrolyticSolution

**IRI:** http://emmo.info/BattINFO#EMMO_fa22874b_76a9_4043_8b8f_6086c88746de

**Definition:** "A liquid electrolyte that consists of solutes dissolved in a solvent."

**Preflabel:** ElectrolyticSolution

**Relations:**

- is_a BattINFO.LiquidElectrolyte

### ElectrochemicalMaterial

**IRI:** http://emmo.info/BattINFO#EMMO_ebdb68e9_c4b5_4d57_a042_c0f51d446755

**Elucidation:** A material that participates in a functional process in an electrochemical assembly.

**Preflabel:** ElectrochemicalMaterial

**Relations:**

- is_a emmo.FunctionalMaterial

### SolidElectrolyte

**IRI:** http://emmo.info/BattINFO#EMMO_0508a114_544a_4f54_a7de_9b947fb4b618

**Definition:** "A solid electrolyte is a solid material where the predominant charge carriers are ions. For example: NASICON (Na Super Ionic Conductor), which has the general formula Na1+xZr2P3-xSix O12 , 0 < x < 3." Pingarron et al., Terminology of electrochemical methods of analysis

**Preflabel:** SolidElectrolyte

**Relations:**

- is_a BattINFO.Electrolyte

## Electrochemical Quantity branch


Figure 3.7: Electrochemical Quantity branch.

### TheoteticalSpecificEnergy

**IRI:** http://emmo.info/BattINFO#EMMO_1c13c786_35ae_4768_88fe_795813d465cd

**Elucidation:** TheoreticalEnergy per unit mass of the cell.

**Physicaldimension:** T-2 L+2 M0 I0 Θ0 N0 J0

**Preflabel:** TheoteticalSpecificEnergy

**Relations:**

- is_a BattINFO.SpecificEnergy

### SpecificEnergy

**IRI:** http://emmo.info/BattINFO#EMMO_ea0c7651_b58b_4caf_ae02_fb6a4dfe6a5d

**Elucidation:** Energy per unit mass.

**Physicaldimension:** T-2 L+2 M0 I0 Θ0 N0 J0

**Preflabel:** SpecificEnergy

**Relations:**

- is_a BattINFO.ElectrochemicalQuantity
- is_a emmo.ISQDerivedQuantity

### TheoreticalStoredEnergy

**IRI:** http://emmo.info/BattINFO#EMMO_9ea6a862_131f_4154_be47_e7417f2fb924

**Elucidation:** Theoretical amount of energy that can be stored in a battery cell. Minimum of the theoretical energy of the positive electrode and negative electrode. Product of the Theoretical Capacity and the Theoretical Open-Circuit Voltage.

**Physicaldimension:** T-2 L+2 M+1 I0 Θ0 N0 J0

**Preflabel:** TheoreticalStoredEnergy

**Relations:**

- is_a BattINFO.StoredEnergy

### StoredEnergy

**IRI:** http://emmo.info/BattINFO#EMMO_4f1ed4ee_06ba_44a4_8ece_1ee56bf12afe

**Elucidation:** Amount of energy stored in a physical object.

**Physicaldimension:** T-2 L+2 M+1 I0 Θ0 N0 J0

**Preflabel:** StoredEnergy

**Relations:**

- is_a BattINFO.ElectrochemicalQuantity
- is_a emmo.InternalEnergy

### ElectrochemicalQuantity

**IRI:** http://emmo.info/BattINFO#EMMO_aecc6094_c6a5_4a36_a825_8a497a2ae112

**Elucidation:** Physical quantities defined within the domain of electrochemistry.

**Preflabel:** ElectrochemicalQuantity

**Relations:**

- is_a emmo.PhysicoChemical

### TheoreticalChargeCapacity

**IRI:** http://emmo.info/BattINFO#EMMO_2b09f961_3374_42e4_8836_bffc6bf522fa

**Elucidation:** Theoretical amount of charge a cell can store. Minimum of the theoretical capacity of the positive electrode and negative electrode.

**Physicaldimension:** T+1 L0 M0 I+1 Θ0 N0 J0

**Preflabel:** TheoreticalChargeCapacity

**Relations:**

- is_a BattINFO.ChargeCapacity

### ChargeCapacity

**IRI:** http://emmo.info/BattINFO#EMMO_791c1915_a791_4450_acd8_7f94764743b5

**Elucidation:** Amount of electric charge that can be stored.

**Physicaldimension:** T+1 L0 M0 I+1 Θ0 N0 J0

**Preflabel:** ChargeCapacity

**Relations:**

- is_a BattINFO.ElectrochemicalQuantity
- is_a emmo.ElectricCharge

### SpecificChargeCapacity

**IRI:** http://emmo.info/BattINFO#EMMO_1e3dc60d_dd6b_47d6_8161_70004fc5ee30

**Elucidation:** Electric charge per unit mass.

**Physicaldimension:** T+1 L0 M-1 I+1 Θ0 N0 J0

**Preflabel:** SpecificChargeCapacity

**Relations:**

- is_a BattINFO.ElectrochemicalQuantity
- is_a emmo.ISQDerivedQuantity

### BatteryQuantity

**IRI:** http://emmo.info/BattINFO#EMMO_230809da_bc18_42ec_ac94_4ca6a86292d1

**Elucidation:** Physical quantities defined within the domain of batteries.

**Preflabel:** BatteryQuantity

**Relations:**

- is_a BattINFO.ElectrochemicalQuantity

### ElectrochemicallyActiveSurfaceArea

**IRI:** http://emmo.info/BattINFO#EMMO_bad1b6f4_1b26_40e2_b552_6d53873e3973

**Elucidation:** The area of the electrode material that is accessible to the electrolyte that is used for charge transfer and/or storage.

**Physicaldimension:** T0 L+2 M0 I0 Θ0 N0 J0

**Preflabel:** ElectrochemicallyActiveSurfaceArea

**Relations:**

- is_a BattINFO.ElectrochemicalQuantity

### ActiveElectrochemicalMaterialLoading

**IRI:** http://emmo.info/BattINFO#EMMO_c955c089_6ee1_41a2_95fc_d534c5cfd3d5

**Elucidation:** Weight of active material in an electrode per unit electrode area.

**Physicaldimension:** T0 L-2 M+1 I0 Θ0 N0 J0

**Preflabel:** ActiveElectrochemicalMaterialLoading

**Relations:**

- is_a BattINFO.ElectrochemicalQuantity

### TheoreticalSpecificCapacity

**IRI:** http://emmo.info/BattINFO#EMMO_8632dee1_0adf_4a47_8400_820b48b86732

**Elucidation:** TheoreticalCapacity divided by the mass of the cell.

**Physicaldimension:** T+1 L0 M-1 I+1 Θ0 N0 J0

**Preflabel:** TheoreticalSpecificCapacity

**Relations:**

- is_a BattINFO.SpecificChargeCapacity

# Electrochemical Transport Quantity branch

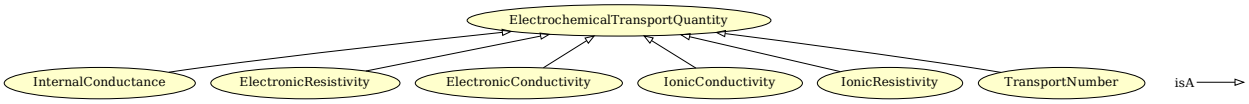


Figure 3.8: Electrochemical Transport Quantity branch.

## InternalConductance

**IRI:** http://emmo.info/BattINFO#EMMO_0c9655c6_6b0b_4819_a219_f286ad196fa9

**Physicaldimension:** T+3 L-2 M-1 I+2 Θ0 N0 J0

**Preflabel:** InternalConductance

**Relations:**

- is_a BattINFO.ElectrochemicalTransportQuantity
- is_a emmo.ElectricConductance

## ElectronicResistivity

**IRI:** http://emmo.info/BattINFO#EMMO_bbcafb37_ceec_436b_bb45_080a2bc656aa

**Elucidation:** Inverse of ElectronicConductivity

**Physicaldimension:** T-3 L+3 M+1 I-2 Θ0 N0 J0

**Preflabel:** ElectronicResistivity

**Relations:**

- is_a emmo.ElectricResistivity
- is_a BattINFO.ElectrochemicalTransportQuantity

## ElectronicConductivity

**IRI:** http://emmo.info/BattINFO#EMMO_6a28741c_ef47_4a11_ba3d_166aef581e86

**Physicaldimension:** T+3 L-3 M-1 I+2 Θ0 N0 J0

**Preflabel:** ElectronicConductivity

**Relations:**

- is_a BattINFO.ElectrochemicalTransportQuantity
- is_a emmo.ElectricConductivity

## ElectrochemicalTransportQuantity

**IRI:** http://emmo.info/BattINFO#EMMO_4a450a27_b84a_4c70_a3a9_15ec30e2f30b

**Elucidation:** An ElectrochemicalQuantity related to the transport of mass and/or charge.

**Preflabel:** ElectrochemicalTransportQuantity

**Relations:**

- is_a BattINFO.ElectrochemicalQuantity

### IonicConductivity

**IRI:** http://emmo.info/BattINFO#EMMO_64e6ed6a_8d17_40ba_937f_f385a54a86c3

**Physicaldimension:** T+3 L-3 M-1 I+2 Θ0 N0 J0

**Preflabel:** IonicConductivity

**Relations:**

- is_a BattINFO.ElectrochemicalTransportQuantity
- is_a emmo.ElectricConductivity

### IonicResistivity

**IRI:** http://emmo.info/BattINFO#EMMO_c90a4ca0_493f_4880_a838_3a2c4b808a03

**Elucidation:** Inverse of IonicConductivity

**Physicaldimension:** T-3 L+3 M+1 I-2 Θ0 N0 J0

**Preflabel:** IonicResistivity

**Relations:**

- is_a BattINFO.ElectrochemicalTransportQuantity
- is_a emmo.ElectricResistivity

### TransportNumber

**IRI:** http://emmo.info/BattINFO#EMMO_5c0ad135_89ea_44da_8df7_f108f8ee1d75

**Elucidation:** Of ions B, the current density due to ions B divided by the sum of current densities of all the ions in the electrolyte.

**Iupacentry:** https://goldbook.iupac.org/terms/view/T06489

**Physicaldimension:** T0 L0 M0 I0 Θ0 N0 J0

**Preflabel:** TransportNumber

**Relations:**

- is_a BattINFO.ElectrochemicalTransportQuantity

## Electrochemical Kinetic Quantity branch

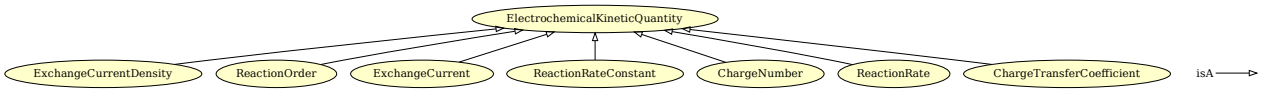


Figure 3.9: Electrochemical Kinetic Quantity branch.

### ExchangeCurrentDensity

**IRI:** http://emmo.info/BattINFO#EMMO_e9fd9ef9_adfe_46cb_b2f9_4558468a25e7

**Elucidation:** Defined by j0 = i0/A, where i0 is the exchange current of the electrode reaction and A is usually taken as the geometric area of the electrode.

**Iupacentry:** https://goldbook.iupac.org/terms/view/M03777

**Physicaldimension:** T0 L-2 M0 I+1 Θ0 N0 J0

**Preflabel:** ExchangeCurrentDensity

**Wikipediaentry:** https://en.wikipedia.org/wiki/Exchange_current_density

**Relations:**

- is_a BattINFO.ElectrochemicalKineticQuantity

## ReactionOrder

**IRI:** http://emmo.info/BattINFO#EMMO_29a57599_aa0d_458f_b23e_666a2da55883

**Elucidation:** If the macroscopic (observed, empirical or phenomenological) rate of reaction (v) for any reaction can be expressed by an empirical differential rate equation (or rate law) which contains a factor of the form k [A]α [B]β … (expressing in full the dependence of the rate of reaction on the concentrations [A], [B] …) where α, β are constant exponents (independent of concentration and time) and k is independent of [A] and [B] etc. (rate constant, rate coefficient), then the reaction is said to be of order α with respect to A, of order β with respect to B, … , and of (total or overall) order n=α+β+… The exponents α, β, … can be positive or negative integral or rational nonintegral numbers.

**Iupacentry:** https://goldbook.iupac.org/terms/view/O04322

**Physicaldimension:** T0 L0 M0 I0 Θ0 N0 J0

**Preflabel:** ReactionOrder

**Relations:**

- is_a BattINFO.ElectrochemicalKineticQuantity

## ExchangeCurrent

**IRI:** http://emmo.info/BattINFO#EMMO_ccde24bb_790a_40ca_a06e_cea156a61031

**Elucidation:** The common value (i0) of the anodic and cathodic partial currents when the reaction is at equilibrium:

i0 = ia = - ic

For an electrode at equilibrium at which only one reaction is significant i = 0. When more than one reaction is significant at a given electrode, subscripts to i0 may be used to distinguish exchange currents. i is not usually zero when only one of these reactions is at equilibrium.

**Iupacentry:** https://goldbook.iupac.org/terms/view/E02238

**Physicaldimension:** T0 L0 M0 I+1 Θ0 N0 J0

**Preflabel:** ExchangeCurrent

**Relations:**

- is_a BattINFO.ElectrochemicalKineticQuantity

## ReactionRateConstant

**IRI:** http://emmo.info/BattINFO#EMMO_dbd808a7_8a8f_43be_9870_02cc35bd1646

**Iupacentry:** https://goldbook.iupac.org/terms/view/O04322

**Preflabel:** ReactionRateConstant

**Relations:**

- is_a BattINFO.ElectrochemicalKineticQuantity

## ChargeNumber

**IRI:** http://emmo.info/BattINFO#EMMO_abfadc99_6e43_4d37_9b04_7fc5b0f327ae

**Elucidation:** Number of electrons transferred in a charge transfer reaction between an electrode and a single entity (ion, radical-ion, or molecule) of an electroactive substance, whose identity must be specified.

-Pingarrón et al.: Terminology of electrochemical methods of analysis, DOI: 10.1515/pac-2018-0109

**Iupacentry:** https://goldbook.iupac.org/terms/view/C00995

**Physicaldimension:** T0 L0 M0 I0 Θ0 N0 J0

**Preflabel:** ChargeNumber

**Relations:**

- is_a BattINFO.ElectrochemicalKineticQuantity

## ReactionRate

**IRI:** http://emmo.info/BattINFO#EMMO_47b7d606_7030_4674_9828_cf83fb4a2995

**Elucidation:** For the general chemical reaction:

aA+bB→pP+qQ+…

occurring under constant-volume conditions, without an appreciable build-up of reaction intermediates, the rate of reaction $\nu$ is defined as:

$\nu$ = -1/a *d[A]/dt* = *-1/b* d[B]/dt = 1/p * d[P]/dt = 1/q * d[Q]/dt

where symbols placed inside square brackets denote amount (or amount of substance) concentrations (conventionally expressed in units of mol dm-3). The symbols R and r are also commonly used in place of $\nu$.

**Iupacentry:** https://goldbook.iupac.org/terms/view/R05156

**Physicaldimension:** T-1 L0 M0 I0 Θ0 N+1 J0

**Preflabel:** ReactionRate

**Wikipediaentry:** https://en.wikipedia.org/wiki/Reaction_rate

**Relations:**

- is_a BattINFO.ElectrochemicalKineticQuantity

## ChargeTransferCoefficient

**IRI:** http://emmo.info/BattINFO#EMMO_a4dfa5c1_55a9_4285_b71d_90cf6613ca31

**Elucidation:** The fraction of the electrostatic potential energy affecting the reduction rate in an electrode reaction, with the remaining fraction affecting the corresponding oxidation rate.

- Guidelli et al.: Transfer coefficient: An assessment, DOI: 10.1515/pac-2014-5026

**Physicaldimension:** T0 L0 M0 I0 Θ0 N0 J0

**Preflabel:** ChargeTransferCoefficient

**Wikipediaentry:** https://en.wikipedia.org/wiki/Charge_transfer_coefficient

**Relations:**

- is_a BattINFO.ElectrochemicalKineticQuantity

### ElectrochemicalKineticQuantity

**IRI:** http://emmo.info/BattINFO#EMMO_21745019_2830_4395_bca7_15ddfd266673

**Elucidation:** An ElectrochemicalQuantity that relates to the kinetics of a reaction.

**Preflabel:** ElectrochemicalKineticQuantity

**Relations:**

- is_a BattINFO.ElectrochemicalQuantity

## Electrochemical Thermodynamic Quantity branch

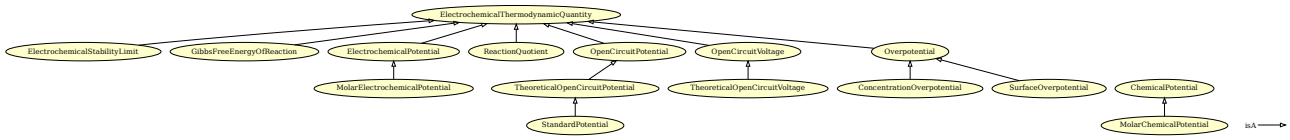


Figure 3.10: Electrochemical Thermodynamic Quantity branch.

### Overpotential

**IRI:** http://emmo.info/BattINFO#EMMO_1cd1d777_e67b_47eb_81f1_edac35d9f2c6

**Elucidation:** Deviation of the potential of an electrode from its equilibrium value required to cause a given current to flow through the electrode.

**Iupacentry:** https://goldbook.iupac.org/terms/view/O04358

**Physicaldimension:** T-3 L+2 M+1 I-1 Θ0 N0 J0

**Preflabel:** Overpotential

**Relations:**

- is_a BattINFO.ElectrochemicalThermodynamicQuantity

### ConcentrationOverpotential

**IRI:** http://emmo.info/BattINFO#EMMO_9ed7210c_c4fa_467b_822d_ba12f885bdf4

**Elucidation:** The concentration overpotential of an electrode reaction at a given electrode current density (c.d.) is basically the difference in equilibrium potentials across the diffusion layer. More precisely, it is the potential of a reference electrode (of the same electrode reaction as the working electrode ) with the interfacial concentrations which establish themselves at c.d., relative to the potential of a similar reference electrode with the concentrations of the bulk solution. From such a measured potential difference, with c.d. flowing, one needs to subtract the ohmic potential drop prevailing between the two electrodes.

**Iupacentry:** https://goldbook.iupac.org/terms/view/C01230

**Physicaldimension:** T-3 L+2 M+1 I-1 Θ0 N0 J0

**Preflabel:** ConcentrationOverpotential

**Relations:**

- is_a BattINFO.Overpotential

## MolarElectrochemicalPotential

**IRI:** http://emmo.info/BattINFO#EMMO_7fe804b8_6126_4132_be8f_b4985d61b1f6

**Elucidation:** ElectrochemicalPotential per mole.

**Iupacentry:** https://goldbook.iupac.org/terms/view/E01945

**Physicaldimension:** T-2 L+2 M+1 I0 Θ0 N-1 J0

**Preflabel:** MolarElectrochemicalPotential

**Relations:**

- is_a BattINFO.ElectrochemicalPotential

## MolarChemicalPotential

**IRI:** http://emmo.info/BattINFO#EMMO_68dc1bf8_9813_43c8_b428_6bd614c3161d

**Elucidation:** ChemicalPotential per mole.

**Physicaldimension:** T-2 L+2 M+1 I0 Θ0 N-1 J0

**Preflabel:** MolarChemicalPotential

**Relations:**

- is_a BattINFO.ChemicalPotential

## ElectrochemicalStabilityLimit

**IRI:** http://emmo.info/BattINFO#EMMO_8f4b90ef_fea4_47c9_99f5_a9b3290a505d

**Elucidation:** Electric potential at which a material undergoes an oxidation or reduction decomposition.

**Example:** For water, the electrochemical stability limits are: Reduction: 0 V Oxidation: 1.23 V

**Physicaldimension:** T-3 L+2 M+1 I-1 Θ0 N0 J0

**Preflabel:** ElectrochemicalStabilityLimit

**Relations:**

- is_a BattINFO.ElectrochemicalThermodynamicQuantity

## TheoreticalOpenCircuitVoltage

**IRI:** http://emmo.info/BattINFO#EMMO_34e440e0_b720_4585_a915_fbe5abb8615d

**Physicaldimension:** T-3 L+2 M+1 I-1 Θ0 N0 J0

**Preflabel:** TheoreticalOpenCircuitVoltage

**Relations:**

- is_a BattINFO.OpenCircuitVoltage

## ChemicalPotential

**IRI:** http://emmo.info/BattINFO#EMMO_17e305af_52a9_4255_a70f_700ba1088f13

**Elucidation:** Energy that can be absorbed or released due to a change of the particle number of the given species

**Iupacentry:** https://goldbook.iupac.org/terms/view/C01032

**Physicaldimension:** T-2 L+2 M+1 I0 Θ0 N0 J0

**Preflabel:** ChemicalPotential

**Wikipediaentry:** https://en.wikipedia.org/wiki/Chemical_potential

**Relations:**

- is_a BattINFO.ElectrochemicalThermodynamicQuantity

### StandardPotential

**IRI:** http://emmo.info/BattINFO#EMMO_7fc10197_41d9_4c1e_a107_928f03eb2d36

**Elucidation:** Theoretical equilibrium potential under standard conditions.

**Physicaldimension:** T-3 L+2 M+1 I-1 Θ0 N0 J0

**Preflabel:** StandardPotential

**Relations:**

- is_a BattINFO.TheoreticalOpenCircuitPotential

### GibbsFreeEnergyOfReaction

**IRI:** http://emmo.info/BattINFO#EMMO_d62ff300_26ac_4b00_bfcd_04a68aff5dc3

**Elucidation:** Change in the Gibbs free energy between the products and reactants in a reaction.

**Physicaldimension:** T-2 L+2 M+1 I0 Θ0 N0 J0

**Preflabel:** GibbsFreeEnergyOfReaction

**Relations:**

- is_a BattINFO.ElectrochemicalThermodynamicQuantity

### ElectrochemicalThermodynamicQuantity

**IRI:** http://emmo.info/BattINFO#EMMO_2d896559_eee3_447c_9759_87c854a4266a

**Elucidation:** A thermodynamically derived ElectrochemicalQuantity.

**Preflabel:** ElectrochemicalThermodynamicQuantity

**Relations:**

- is_a BattINFO.ElectrochemicalQuantity

### TheoreticalOpenCircuitPotential

**IRI:** http://emmo.info/BattINFO#EMMO_d91940f0_c8b6_4505_9b68_6bf6cfc5c544

**Elucidation:** Theoretical electrode potential considering a given electrochemical charge-transfer reaction.

**Physicaldimension:** T-3 L+2 M+1 I-1 Θ0 N0 J0

**Preflabel:** TheoreticalOpenCircuitPotential

**Relations:**

- is_a BattINFO.OpenCircuitPotential

### ElectrochemicalPotential

**IRI:** http://emmo.info/BattINFO#EMMO_1422cde1_929e_46b6_b0dc_1010eebc5dfd

**Iupacentry:** https://goldbook.iupac.org/terms/view/E01945

**Physicaldimension:** T-2 L+2 M+1 I0 Θ0 N0 J0

**Preflabel:** ElectrochemicalPotential

**Relations:**

- is_a BattINFO.ElectrochemicalThermodynamicQuantity

### ReactionQuotient

**IRI:** http://emmo.info/BattINFO#EMMO_740d5817_3fa7_464a_90c3_55552e51a3df

**Physicaldimension:** T0 L0 M0 I0 Θ0 N0 J0

**Preflabel:** ReactionQuotient

**Wikipediaentry:** https://en.wikipedia.org/wiki/Reaction_quotient

**Relations:**

- is_a BattINFO.ElectrochemicalThermodynamicQuantity

### OpenCircuitPotential

**IRI:** http://emmo.info/BattINFO#EMMO_9c657fdc_b9d3_4964_907c_f9a6e8c5f52b

**Elucidation:** Measured electric potential of an electrode without external current flow.

**Physicaldimension:** T-3 L+2 M+1 I-1 Θ0 N0 J0

**Preflabel:** OpenCircuitPotential

**Relations:**

- is_a BattINFO.ElectrochemicalThermodynamicQuantity
- is_a emmo.ElectricPotential

### SurfaceOverpotential

**IRI:** http://emmo.info/BattINFO#EMMO_60741c58_a10d_4aa6_bb68_0066a6ff8e30

**Elucidation:** The potential of a working electrode relative to a reference electrode of the same kinds placed in the solution adjacent to the surface of the working electrode (just outside the double layer).

**Physicaldimension:** T-3 L+2 M+1 I-1 Θ0 N0 J0

**Preflabel:** SurfaceOverpotential

**Relations:**

- is_a BattINFO.Overpotential

### OpenCircuitVoltage

**IRI:** http://emmo.info/BattINFO#EMMO_0c0c623c_43b8_426d_a536_168108e2353a

**Elucidation:** Measured difference between two electrodes without external current flow.

**Physicaldimension:** T-3 L+2 M+1 I-1 Θ0 N0 J0

**Preflabel:** OpenCircuitVoltage

**Relations:**

- is_a emmo.ElectricPotential
- is_a BattINFO.ElectrochemicalThermodynamicQuantity

### TheoreticalOpenCircuitVoltage

**IRI:** http://emmo.info/BattINFO#EMMO_367a4916_d03a_483c_9f2c_6588370fc9d9

**Elucidation:** Difference between the theoretical electric potentials of the positive electrode and negeative electrode under no current flow.

**Physicaldimension:** T-3 L+2 M+1 I-1 Θ0 N0 J0

**Preflabel:** TheoreticalOpenCircuitVoltage

**Relations:**

- is_a BattINFO.OpenCircuitVoltage

# Chapter 4

# Appendix

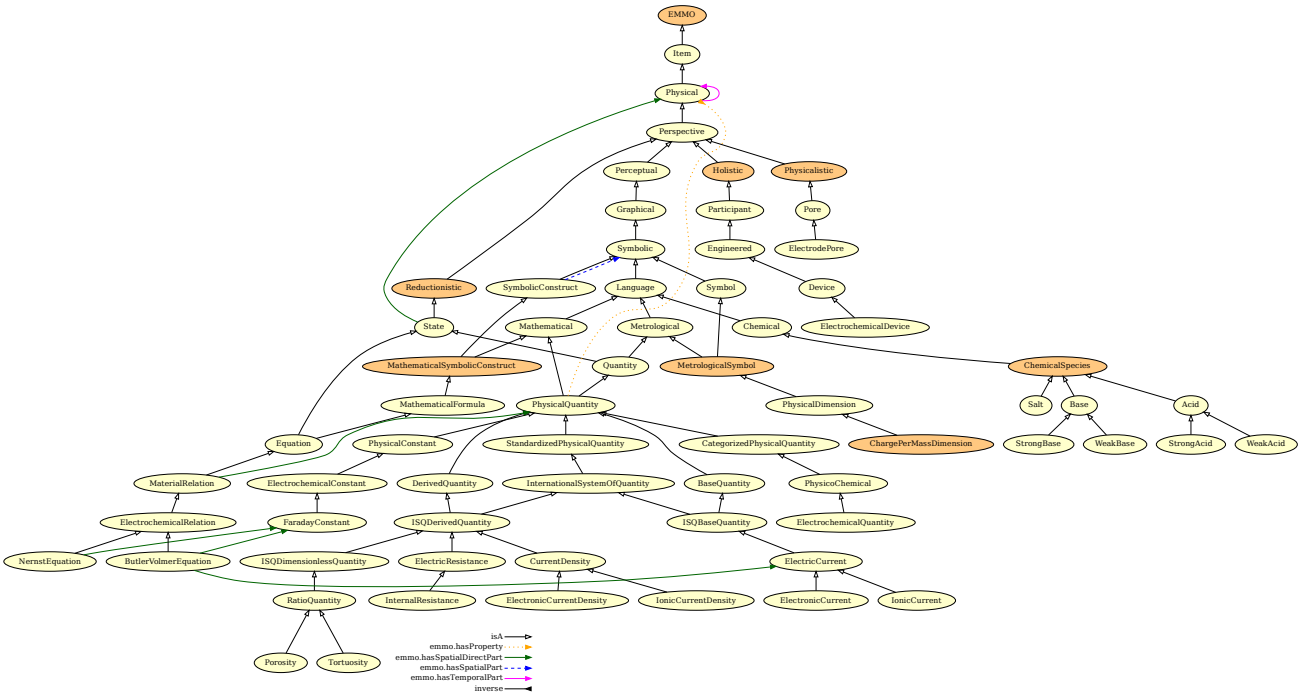


Figure 4.1: All classes defined with the BattINFO namespace. In addition parent classes belonging to EMMO are included.