Battery INterFace Ontology (BattINFO) Reference Documentation

VERSION 0.0.1

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



February 27, 2021

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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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.

It is released under the Creative Commons Attribution 4.0 International license (CC BY 4.0).

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

 $\textbf{IRI:} \ \text{http://emmo.info/emmo\#EMMO_038e37a3_1684_4980_b5e4_67ab34cd5bdb}$

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

Preflabel: ActiveParticipant

Relations:

ullet is_a emmo.Participant

• Inverse(emmo.hasProperParticipant) some emmo.FunctionalProcess

Functional Material

 $\textbf{IRI:} \ \text{http://emmo.info/emmo\#EMMO_d95e6e0d-e8eb-411a-b407-0d1a517e8767}$

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.

 ${\bf Preflabel:} \ {\bf Functional Process}$

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:

- \bullet 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

Physical dimension: T0 L0 M0 I0 Θ -1 N0 J0

 ${\bf Preflabel:}\ Volumetric Thermal Expansion Coefficient$

• 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.

Physical dimension: T-1 L+2 M0 I0 Θ 0 N-1 J0

Preflabel: SingleComponentDiffusivity

Relations:

is_a emmo.ISQDerivedQuantity is_a emmo.PhysicoChemical

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.

Physical dimension: T-1 L+2 M0 I0 Θ 0 N-1 J0

Preflabel: SingleComponentDiffusivity

Relations:

is_a emmo.ISQDerivedQuantity is a emmo.PhysicoChemical

${\bf Single Component Maximal Diffusivity}$

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.PhysicoChemicalis a emmo.ISQDerivedQuantity

SingleComponentActivationEnergyOfDiffusion

 $\textbf{IRI:} \ \text{http://emmo.info/emmo\#EMMO_2f761aff_88d1_4e79_a85e_09d6f400de56} \\ \textbf{IRI:} \ \text{IRI:} \ \text{$

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

Physical dimension: T-2 L+2 M+1 I0 Θ 0 N0 J0

Preflabel: SingleComponentActivationEnergyOfDiffusion

Relations:

• is a emmo.PhysicoChemical

• is_a emmo.Energy

MolarHeatCapacity

 $\textbf{IRI:} \ http://emmo.info/emmo\#EMMO_50c5d440_683c_400f_909e_b03c0327de9c$

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

Physical dimension: T-2 L+2 M+1 I0 Θ -1 N-1 J0

Preflabel: MolarHeatCapacity

Relations:

is_a emmo.PhysicoChemical is_a emmo.ISQDerivedQuantity

EnergyDensity

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

Elucidation: Energy per unit volume.

Physical dimension: T-2 L+2 M+1 I0 $\Theta0~\mathrm{N0}~\mathrm{J0}$

Preflabel: EnergyDensity

Relations:

• is a emmo.ISQDerivedQuantity

ThermalExpansionCoefficient

 $\textbf{IRI:} \ \text{http://emmo.info/emmo\#EMMO_7684ddff_d99b_405d_aad2_90e830b8403c}$

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

 ${\bf Preflabel:}\ {\bf Thermal Expansion Coefficient}$

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.

Physical dimension: T-2 L+2 M+1 I0 Θ -1 N0 J0

Preflabel: HeatCapacity

Relations:

is_a emmo.PhysicoChemical is_a emmo.ISQDerivedQuantity

ThermalConductivity

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

Elucidation: The ability of a material to conduct heat.

Physical dimension: T-3 L+1 M+1 I0 Θ -1 N0 J0

Preflabel: ThermalConductivity

Relations:

is_a emmo.PhysicoChemical is_a emmo.ISQDerivedQuantity

SpecificHeatCapacity

 $\textbf{IRI:} \ \text{http://emmo.info/emmo\#EMMO_b4f4ed28_d24c_4a00_9583_62ab839abeca}$

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.

Physical dimension: T-2 L+2 M0 I0 $\Theta\text{-}1$ N0 J0

Preflabel: SpecificHeatCapacity

Relations:

is_a emmo.PhysicoChemical is_a emmo.ISQDerivedQuantity

Additional quantity dimensions

PerTemperatureDimension

IRI: http://emmo.info/emmo#EMMO 6e9aef15 272b 4eea aaa9 2f38b8ae951f

 $\textbf{Preflabel:} \ \operatorname{PerTemperatureDimension}$

- $\bullet \;$ is_a emmo.PhysicalDimension
- equivalent_to emmo.has Symbol
Data value "T0 L0 M0 I0 $\Theta\text{-}1$ 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

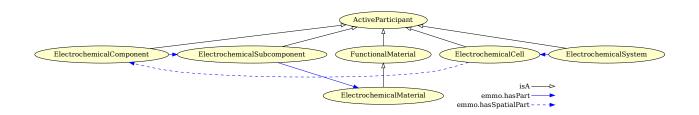


Figure 3.1: Active Participant branch.

ActiveParticipant

 $\textbf{IRI:} \ \text{http://emmo.info/emmo\#EMMO_038e37a3_1684_4980_b5e4_67ab34cd5bdb}$

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

Functional Material

 $\textbf{IRI:} \ \text{http://emmo.info/emmo\#EMMO_d95e6e0d-e8eb-411a-b407-0d1a517e8767}$

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

- is_a emmo.ActiveParticipant
- is_a emmo.Material

Electrochemical System branch



Figure 3.2: Electrochemical System branch.

ElectrochemicalSystem

 $\textbf{IRI:} \ \text{http://emmo.info/BattINFO\#EMMO_4e4d7f4b-680b-469e-bdd4-728dd3e465bf}$

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

Preflabel: ElectrochemicalSystem

Relations:

• is a emmo. Active Participant

 $\bullet \ \ emmo. has Part \ some \ BattINFO. Electrochemical Cell$

Electrochemical Cell branch

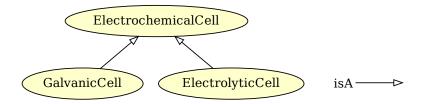


Figure 3.3: Electrochemical Cell branch.

GalvanicCell

 $\textbf{IRI:} \ \text{http://emmo.info/BattINFO\#EMMO_e248373f_294f_4ca4_9edf_0ad6653bb64f}$

Elucidation: An electrochemical cell that spontaneously produces work.

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

Preflabel: GalvanicCell

Relations:

 $\bullet \ \ is_a \ BattINFO. Electrochemical Cell$

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.Object
- is a emmo. Active Participant
- is a emmo.Matter
- emmo.hasConventionalQuantity some BattINFO.OpenCircuitVoltage
- emmo.hasConventionalQuantity some emmo.ThermalConductivity
- emmo.hasConventionalQuantity some emmo.EnergyDensity
- emmo.hasConventionalQuantity some emmo.ThermodynamicTemperature
- emmo.hasConventionalQuantity some emmo.Volume
- emmo.hasConventionalQuantity some BattINFO.StoredEnergy
- emmo.hasConventionalQuantity some emmo.Density
- emmo.hasConventionalQuantity some emmo.HeatCapacity
- emmo.hasConventionalQuantity some emmo.SpecificHeatCapacity
- emmo.hasConventionalQuantity some emmo.ThermalExpansionCoefficient
- emmo.hasConventionalQuantity some emmo.ElectricPotential
- emmo.hasConventionalQuantity some BattINFO.InternalConductance
- $\bullet \ \ emmo. has Conventional Quantity \ some \ emmo. Electric Impedance$
- emmo.hasConventionalQuantity some BattINFO.ChargeCapacity
- emmo.hasConventionalQuantity some BattINFO.SpecificEnergy
- emmo.hasConventionalQuantity some BattINFO.InternalResistance
- emmo.hasSpatialPart some BattINFO.ElectrochemicalComponent
- emmo.hasConventionalQuantity some emmo.Mass
- emmo.hasConventionalQuantity some BattINFO.SpecificChargeCapacity

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

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

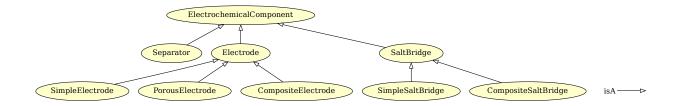


Figure 3.4: Electrochemical Component branch.

Preflabel: SaltBridge

Relations:

 $\bullet \ \ is_a \ BattINFO. Electrochemical Component$

SimpleElectrode

 $\textbf{IRI:} \ \text{http://emmo.info/BattINFO\#EMMO_029f0b45-70a7-481f-8154-bf982a77e08c}$

Elucidation: An electrode consisting of a single ElectrochemicalSubComponent

Example: Metal foil.

Preflabel: SimpleElectrode

Relations:

• is_a BattINFO.Electrode

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:

 $\bullet \;$ is_a emmo. Active
Participant

• 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.

 ${\bf Preflabel:} \ {\bf Simple Salt Bridge}$

Relations:

- \bullet is_a emmo.State
- is a BattINFO.SaltBridge
- emmo.hasSpatialDirectPart exactly 1 BattINFO.IonicSubcomponent

Separator

 $\textbf{IRI:} \ \text{http://emmo.info/BattINFO\#EMMO}_331e6cca_f260_4bf8_af55_35304fe1bbe0$

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:

 \bullet is_a BattINFO.ElectrochemicalComponent

PorousElectrode

 $\textbf{IRI:} \ \text{http://emmo.info/BattINFO\#EMMO}_3663991d-9319-4f7a-922b-f0e428b58801$

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

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

Composite Salt Bridge

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
- $\bullet \hspace{0.2cm} \textbf{emmo.hasSpatialDirectPart} \hspace{0.2cm} \textbf{min} \hspace{0.1cm} 2 \hspace{0.1cm} \textbf{BattINFO.ElectrochemicalSubcomponent}$
- $\bullet \ \ emmo. has Spatial Direct Part \ some \ BattINFO. Ionic Subcomponent$

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

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

Electrochemical Subcomponent branch

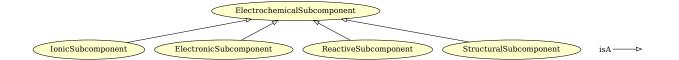


Figure 3.5: Electrochemical Subcomponent branch.

IonicSubcomponent

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

Preflabel: IonicSubcomponent

Relations:

• is a BattINFO.ElectrochemicalSubcomponent

ElectronicSubcomponent

 $\textbf{IRI:} \ http://emmo.info/BattINFO\#EMMO_9c4e61c6-4a7b-41c2-9133-e780e144ddcd$

Elucidation: An ElectrochemicalSubcomponent whose primary role is electronic

Example: Current Collector Conducting Additive

Preflabel: ElectronicSubcomponent

Relations:

 \bullet is_a BattINFO.ElectrochemicalSubcomponent

ReactiveSubcomponent

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

Elucidation: An Electrochemical Subcomponent whose primary role is to participate in a reaction.

Preflabel: ReactiveSubcomponent

Relations:

• is_a BattINFO.ElectrochemicalSubcomponent

ElectrochemicalSubcomponent

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

Elucidation: A subcomponent of an Electrochemical Component.

Preflabel: ElectrochemicalSubcomponent

Relations:

• is_a emmo.ActiveParticipant

• emmo.hasPart some BattINFO.ElectrochemicalMaterial

StructuralSubcomponent

 $\textbf{IRI:} \ \text{http://emmo.info/BattINFO\#EMMO_dd15b4b0-11e7-4900-b379-9702a8caa6bb}$

Preflabel: StructuralSubcomponent

Relations:

 \bullet is_a BattINFO. ElectrochemicalSubcomponent

Electrochemical Material branch

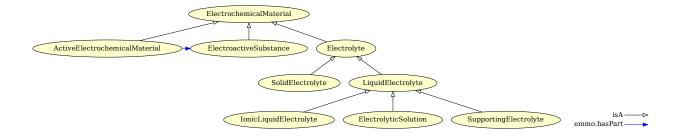


Figure 3.6: Electrochemical Material branch.

LiquidElectrolyte

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

Definition: "An electrolyte in the liquid phase"

 $\textbf{Preflabel:} \ \text{LiquidElectrolyte}$

Relations:

• is_a BattINFO.Electrolyte

ActiveElectrochemicalMaterial

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

 ${\bf Preflabel:} \ {\bf Active Electrochemical Material}$

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:

 \bullet 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

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

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

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

Electrolytic Solution

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

SupportingElectrolyte

 $\textbf{IRI:} \ \text{http://emmo.info/BattINFO\#EMMO_1fc5642c_b7b2_43bf_ad20_f96001db8800}$

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

Electrochemical Quantity branch



Figure 3.7: Electrochemical Quantity branch.

Battery Quantity

Elucidation: Physical quantities defined within the domain of batteries.

Preflabel: BatteryQuantity

Relations:

• is_a BattINFO.ElectrochemicalQuantity

StoredEnergy

 $\textbf{IRI:} \ \text{http://emmo.info/BattINFO\#EMMO_4f1ed4ee_06ba_44a4_8ece_1ee56bf12afe}$

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 emmo.InternalEnergy

• is a BattINFO.ElectrochemicalQuantity

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.

Physical dimension: T-2 L+2 M+1 I0 $\Theta 0$ N0 J0

Preflabel: TheoreticalStoredEnergy

• is_a BattINFO.StoredEnergy

TheoreticalSpecificCapacity

 $\textbf{IRI:} \ \text{http://emmo.info/BattINFO\#EMMO} \underline{8632} \\ \text{dee1} \underline{-0} \\ \text{adf} \underline{-4} \\ \text{a47} \underline{-8400} \underline{-820} \\ \text{b48b86732} \\ \text{info/BattINFO\#EMMO} \underline{-8632} \\ \text{dee1} \underline{-0} \\ \text{adf} \underline{-4} \\ \text{a47} \underline{-8400} \underline{-820} \\ \text{b48b86732} \\ \text{info/BattINFO\#EMMO} \underline{-8632} \\ \text{dee1} \underline{-0} \\ \text{adf} \underline{-4} \\ \text{a47} \underline{-8400} \underline{-820} \\ \text{b48b86732} \\ \text{info/BattINFO\#EMMO} \underline{-8632} \\ \text{dee1} \underline{-0} \\ \text{adf} \underline{-4} \\ \text{a47} \underline{-8400} \underline{-820} \\ \text{b48b86732} \\ \text{info/BattINFO\#EMMO} \underline{-8632} \\ \text{dee1} \underline{-0} \\ \text{adf} \underline{-4} \\ \text{a47} \underline{-8400} \underline{-820} \\ \text{b48b86732} \\ \text{dee1} \underline{-0} \\ \text{adf} \underline{-4} \\ \text{a47} \underline{-8400} \underline{-820} \\ \text{b48b86732} \\ \text{dee1} \underline{-0} \\ \text{adf} \underline{-4} \\ \text{a47} \underline{-8400} \underline{-820} \\ \text{b48b86732} \\ \text{dee1} \underline{-0} \\ \text{adf} \underline{-4} \\ \text{a47} \underline{-8400} \underline{-820} \\ \text{b48b86732} \\ \text{dee1} \underline{-0} \\ \text{adf} \underline{-4} \\ \text{a47} \underline{-8400} \underline{-820} \\ \text{b48b86732} \\ \text{dee1} \\ \text{adf} \underline{-0} \\$

Elucidation: TheoreticalCapacity divided by the mass of the cell.

Physical dimension: T+1 L0 M-1 I+1 Θ 0 N0 J0

Preflabel: Theoretical Specific Capacity

Relations:

 $\bullet \ \ {\rm is_a\ BattINFO.SpecificChargeCapacity}$

ChargeCapacity

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

Elucidation: Amount of electric charge that can be stored.

Physical dimension: T+1 L0 M0 I+1 Θ 0 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.

Physical dimension: T+1 L0 M-1 I+1 Θ 0 N0 J0

Preflabel: SpecificChargeCapacity

Relations:

• is_a emmo.ISQDerivedQuantity

• is_a BattINFO.ElectrochemicalQuantity

SpecificEnergy

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

Elucidation: Energy per unit mass.

Physical dimension: T-2 L+2 M0 I0 Θ 0 N0 J0

Preflabel: SpecificEnergy

Relations:

• is_a BattINFO.ElectrochemicalQuantity

• is_a emmo.ISQDerivedQuantity

ActiveElectrochemicalMaterialLoading

IRI: http://emmo.info/BattINFO#EMMO c955c089 6ee1 41a2 95fc d534c5cfd3d5

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

Physical dimension: T0 L-2 M+1 I0 Θ 0 N0 J0 Preflabel: Active Electrochemical Material Loading

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

TheoteticalSpecificEnergy

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

Elucidation: TheoreticalEnergy per unit mass of the cell.

Physical dimension: T-2 L+2 M0 I0 Θ 0 N0 J0

Preflabel: TheoteticalSpecificEnergy

Relations:

• is_a BattINFO.SpecificEnergy

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.

Physical dimension: T+1 L0 M0 I+1 Θ0 N0 J0

 ${\bf Preflabel:}\ {\bf Theoretical Charge Capacity}$

Relations:

• is_a BattINFO.ChargeCapacity

ElectrochemicalQuantity

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

Elucidation: Physical quantities defined within the domain of electrochemistry.

Preflabel: Electrochemical Quantity

Relations:

• is_a emmo.PhysicoChemical

Electrochemical Transport Quantity branch

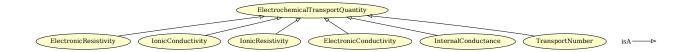


Figure 3.8: Electrochemical Transport Quantity branch.

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 BattINFO.ElectrochemicalTransportQuantity

• is a emmo. Electric Resistivity

ElectrochemicalTransportQuantity

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

Elucidation: An Electrochemical Quantity 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

Physical dimension: T+3 L-3 M-1 I+2 $\Theta 0$ N0 J0

Preflabel: IonicConductivity

Relations:

 $\bullet \ \ is_a \ emmo. Electric Conductivity$

 $\bullet \ \ is_a \ BattINFO. Electrochemical Transport Quantity$

IonicResistivity

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

Elucidation: Inverse of IonicConductivity

Physical dimension: T-3 L+3 M+1 I-2 $\Theta 0$ N0 J0

Preflabel: IonicResistivity

Relations:

• is_a emmo.ElectricResistivity

• is_a BattINFO.ElectrochemicalTransportQuantity

Electronic Conductivity

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

Physical dimension: T+3 L-3 M-1 I+2 $\Theta 0$ N0 J0

Preflabel: ElectronicConductivity

Relations:

• is a emmo. Electric Conductivity

• is a BattINFO.ElectrochemicalTransportQuantity

InternalConductance

IRI: http://emmo.info/BattINFO#EMMO 0c9655c6 6b0b 4819 a219 f286ad196fa9

Physical dimension: T+3 L-2 M-1 I+2 $\Theta 0$ N0 J0

Preflabel: InternalConductance

Relations:

• is_a BattINFO.ElectrochemicalTransportQuantity

• is a emmo. Electric Conductance

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

Physical dimension: T0 L0 M0 I0 Θ 0 N0 J0

Preflabel: TransportNumber

Relations:

• is a BattINFO.ElectrochemicalTransportQuantity

Electrochemical Kinetic Quantity branch

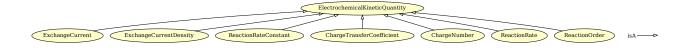


Figure 3.9: Electrochemical Kinetic Quantity branch.

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

Physical dimension: T0 L0 M0 I+1 Θ 0 N0 J0

Preflabel: ExchangeCurrent

Relations:

• is_a BattINFO.ElectrochemicalKineticQuantity

ElectrochemicalKineticQuantity

IRI: http://emmo.info/BattINFO#EMMO 21745019 2830 4395 bca7 15ddfd266673

Elucidation: An Electrochemical Quantity that relates to the kinetics of a reaction.

Preflabel: ElectrochemicalKineticQuantity

Relations:

• is_a BattINFO.ElectrochemicalQuantity

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 Θ 0 N0 J0

Preflabel: ExchangeCurrentDensity

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

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

ChargeTransferCoefficient

 $\textbf{IRI:} \ \text{http://emmo.info/BattINFO\#EMMO_a4dfa5c1_55a9_4285_b71d_90cf6613ca31}$

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

Physical dimension: T0 L0 M0 I0 Θ 0 N0 J0

Preflabel: ChargeTransferCoefficient

Wikipediaentry: https://en.wikipedia.org/wiki/Charge transfer coefficient

• 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

Physical dimension: T0 L0 M0 I0 $\Theta0$ 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:

 $aA+bB\rightarrow pP+qQ+...$

occurring under constant-volume conditions, without an appreciable build-up of reaction intermediates, the rate of reaction ν 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 ν .

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

Physicaldimension: T-1 L0 M0 I0 Θ 0 N+1 J0

Preflabel: ReactionRate

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

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 $[A]\alpha$ $[B]\beta$... (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 $n=\alpha+\beta+...$ The exponents α , β , ... can be positive or negative integral or rational nonintegral numbers.

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

Physical dimension: T0 L0 M0 I0 $\Theta 0$ N0 J0

Preflabel: ReactionOrder

Relations:

• is_a BattINFO.ElectrochemicalKineticQuantity

Electrochemical Thermodynamic Quantity branch

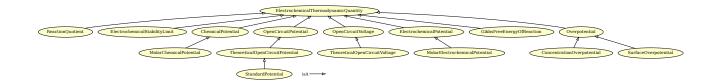


Figure 3.10: Electrochemical Thermodynamic Quantity branch.

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

Physical dimension: T-3 L+2 M+1 I-1 $\Theta 0$ N0 J0

Preflabel: Overpotential

Relations:

 $\bullet \ \ is_a \ BattINFO. Electrochemical Thermodynamic Quantity$

ReactionQuotient

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

Physical dimension: T0 L0 M0 I0 Θ 0 N0 J0

Preflabel: ReactionQuotient

 $\textbf{Wikipedia} entry: \ \text{https://en.wikipedia.org/wiki/Reaction_quotient}$

Relations:

 \bullet is_a BattINFO.ElectrochemicalThermodynamicQuantity

MolarChemicalPotential

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

Elucidation: ChemicalPotential per mole.

Physical dimension: T-2 L+2 M+1 I0 $\Theta 0$ N-1 J0

Preflabel: MolarChemicalPotential

Relations:

 \bullet 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

Physical dimension: T-3 L+2 M+1 I-1 Θ 0 N0 J0

Preflabel: ElectrochemicalStabilityLimit

Relations:

 $\bullet \ \ is_a \ BattINFO. Electrochemical Thermodynamic Quantity$

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

Physical dimension: T-3 L+2 M+1 I-1 Θ 0 N0 J0

Preflabel: ConcentrationOverpotential

Relations:

• is a BattINFO.Overpotential

StandardPotential

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

Elucidation: Theoretical equilibrium potential under standard conditions.

Physical dimension: T-3 L+2 M+1 I-1 Θ 0 N0 J0

Preflabel: StandardPotential

Relations:

• is_a BattINFO.TheoreticalOpenCircuitPotential

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

Physical dimension: T-2 L+2 M+1 I0 $\Theta0~\mathrm{N0}~\mathrm{J0}$

Preflabel: ChemicalPotential

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

Relations:

 \bullet is_a BattINFO.ElectrochemicalThermodynamicQuantity

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).

Physical dimension: T-3 L+2 M+1 I-1 Θ 0 N0 J0

Preflabel: SurfaceOverpotential

Relations:

• is_a BattINFO.Overpotential

TheoreticalOpenCircuitVoltage

 $\textbf{IRI:} \ \text{http://emmo.info/BattINFO\#EMMO}_34e440e0_b720_4585_a915_fbe5abb8615d$

Physical dimension: T-3 L+2 M+1 I-1 Θ 0 N0 J0

Preflabel: TheoreticalOpenCircuitVoltage

Relations:

• is_a BattINFO.OpenCircuitVoltage

Theoretical Open Circuit Potential

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

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

Physical dimension: T-3 L+2 M+1 I-1 Θ 0 N0 J0

Preflabel: TheoreticalOpenCircuitPotential

Relations:

 $\bullet \ \ is_a \ BattINFO.OpenCircuitPotential$

MolarElectrochemicalPotential

 $\textbf{IRI:} \ \text{http://emmo.info/BattINFO\#EMMO_7fe804b8_6126_4132_be8f_b4985d61b1f6}$

Elucidation: ElectrochemicalPotential per mole.

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

Physical dimension: T-2 L+2 M+1 I0 $\Theta 0$ N-1 J0

Preflabel: MolarElectrochemicalPotential

Relations:

• is a BattINFO.ElectrochemicalPotential

OpenCircuitPotential

 $\textbf{IRI:} \ \text{http://emmo.info/BattINFO\#EMMO_9c657fdc_b9d3_4964_907c_f9a6e8c5f52b}$

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

Physical dimension: T-3 L+2 M+1 I-1 Θ 0 N0 J0

Preflabel: OpenCircuitPotential

Relations:

 \bullet is_a BattINFO.ElectrochemicalThermodynamicQuantity

 \bullet is_a emmo. ElectricPotential

OpenCircuitVoltage

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

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

Physical dimension: T-3 L+2 M+1 I-1 Θ 0 N0 J0

Preflabel: OpenCircuitVoltage

Relations:

 \bullet is_a BattINFO.ElectrochemicalThermodynamicQuantity

 \bullet is_a emmo.ElectricPotential

Theoretical Open Circuit Voltage

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.

Physical dimension: T-3 L+2 M+1 I-1 Θ 0 N0 J0

Preflabel: TheoreticalOpenCircuitVoltage

Relations:

• is_a BattINFO.OpenCircuitVoltage

Electrochemical Potential

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

 $\textbf{Iupacentry:}\ \text{https://goldbook.iupac.org/terms/view/E01945}$

Physical dimension: T-2 L+2 M+1 I0 Θ0 N0 J0

Preflabel: ElectrochemicalPotential

Relations:

 \bullet is_a BattINFO.ElectrochemicalThermodynamicQuantity

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.

Physical dimension: T-2 L+2 M+1 I0 Θ0 N0 J0

Preflabel: GibbsFreeEnergyOfReaction

Relations:

• is a BattINFO.ElectrochemicalThermodynamicQuantity

${\bf Electrochemical Thermodynamic Quantity}$

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

Elucidation: A thermodynamically derived ElectrochemicalQuantity.

Preflabel: ElectrochemicalThermodynamicQuantity

Relations:

• is_a BattINFO.ElectrochemicalQuantity

Chapter 4

Appendix

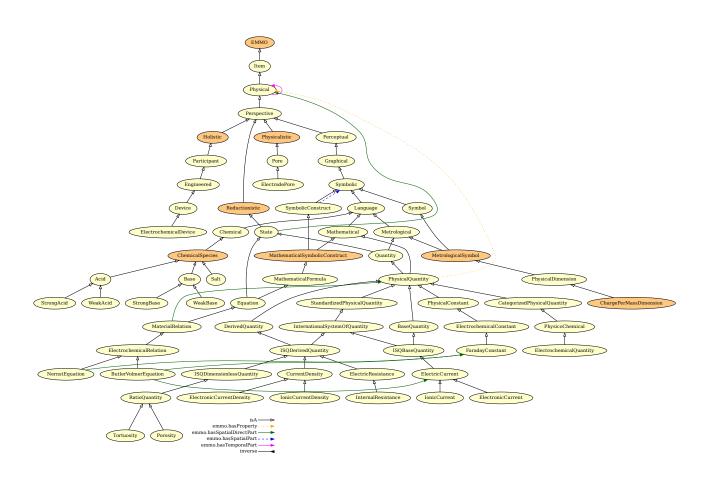


Figure 4.1: All classes defined with the BattINFO name space. In addition parent classes belonging to EMMO are included.