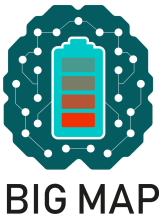
Battery INterFace Ontology (BattINFO) Reference Documentation

Version 0.0.1

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



February 26, 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.

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

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.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.

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

Preflabel: SingleComponentDiffusivity

Relations:

- is_a emmo.ISQDerivedQuantity
- is_a emmo.PhysicoChemical

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.Energy
- is_a emmo.PhysicoChemical

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.PhysicoChemical
- is_a emmo.ISQDerivedQuantity

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.PhysicoChemical
- is_a emmo.ISQDerivedQuantity

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.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.

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

Preflabel: ThermalConductivity

Relations:

- is_a emmo.PhysicoChemical
- is_a emmo.ISQDerivedQuantity

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.PhysicoChemical
- is_a emmo.ISQDerivedQuantity

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

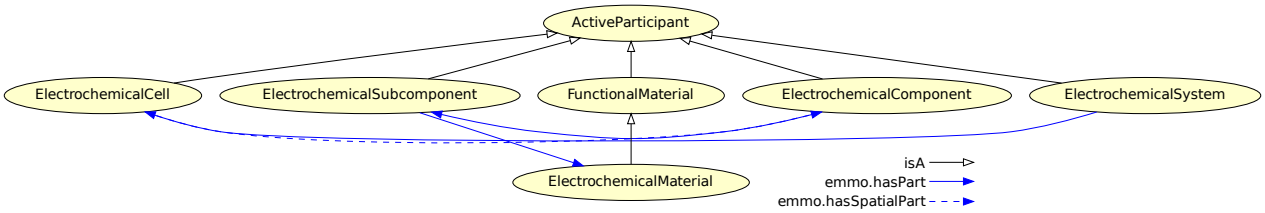

Figure 3.1: Active Participant branch.

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

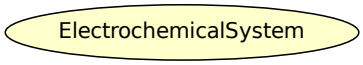

Figure 3.2: Electrochemical System branch.

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

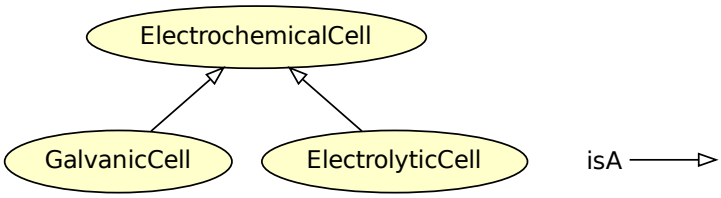

Figure 3.3: Electrochemical Cell branch.

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

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

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

Electrochemical Component branch

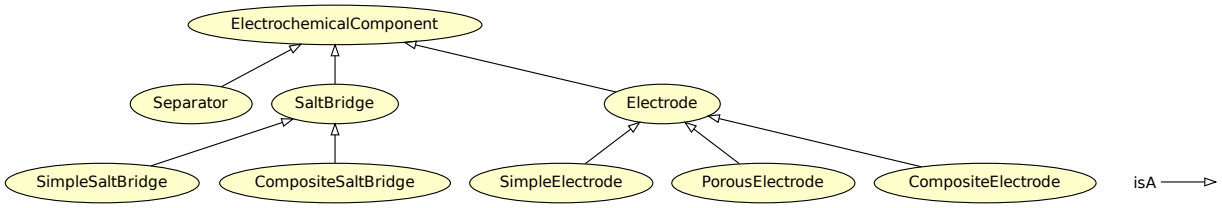

Figure 3.4: Electrochemical Component branch.

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:

- is_a BattINFO.ElectrochemicalComponent

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

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

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

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

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

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

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

Electrochemical Subcomponent branch

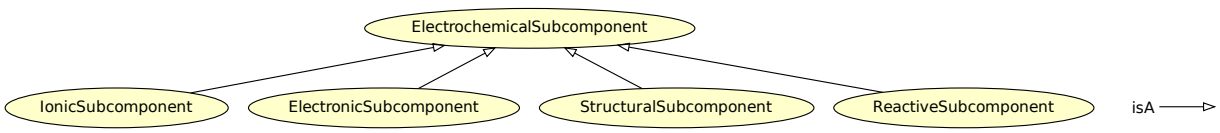

Figure 3.5: Electrochemical Subcomponent branch.

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

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

StructuralSubcomponent

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

Preflabel: StructuralSubcomponent

Relations:

- is_a BattINFO.ElectrochemicalSubcomponent

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

ElectroactiveSubstance

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

Preflabel: ElectroactiveSubstance

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

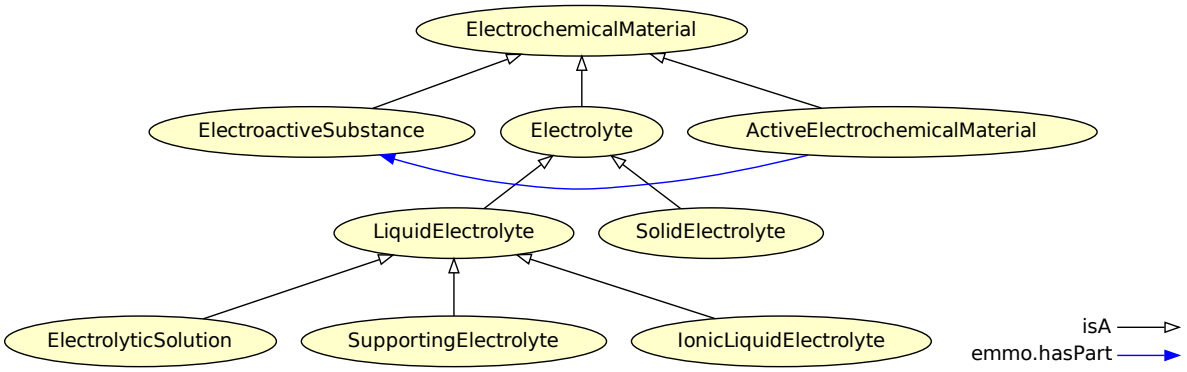

Figure 3.6: Electrochemical Material branch.

LiquidElectrolyte

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

Definition: "An electrolyte in the liquid phase"

Preflabel: LiquidElectrolyte

Relations:

- is_a BattINFO.Electrolyte

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

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

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

ActiveElectrochemicalMaterial

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

Preflabel: ActiveElectrochemicalMaterial

Relations:

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

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

Electrochemical Quantity branch

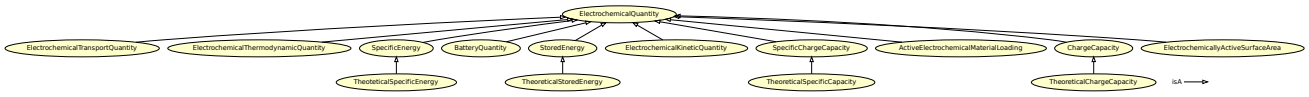

Figure 3.7: Electrochemical Quantity branch.

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

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

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

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

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

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

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 emmo.InternalEnergy
- 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

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

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

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

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

Electrochemical Transport Quantity branch

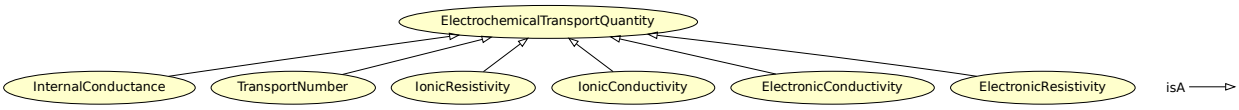

Figure 3.8: Electrochemical Transport Quantity branch.

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

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

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

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 emmo.ElectricResistivity
- is_a BattINFO.ElectrochemicalTransportQuantity

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 emmo.ElectricConductivity
- 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 emmo.ElectricConductivity
- is_a BattINFO.ElectrochemicalTransportQuantity

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

Electrochemical Kinetic Quantity branch

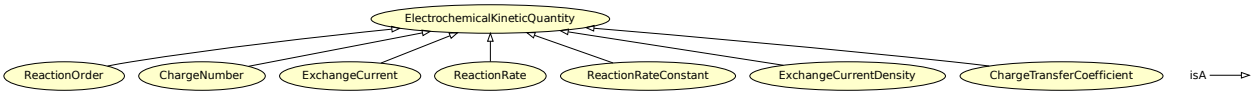

Figure 3.9: Electrochemical Kinetic Quantity branch.

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

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

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

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

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 ν is defined as:

ν = -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 Θ0 N+1 J0

Preflabel: ReactionRate

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

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

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

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

Electrochemical Thermodynamic Quantity branch

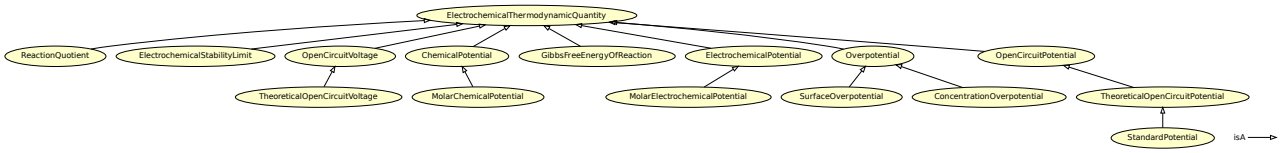

Figure 3.10: Electrochemical Thermodynamic Quantity branch.

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

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

ElectrochemicalThermodynamicQuantity

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

Elucidation: A thermodynamically derived ElectrochemicalQuantity.

Preflabel: ElectrochemicalThermodynamicQuantity

Relations:

- is_a BattINFO.ElectrochemicalQuantity

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

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

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

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 BattINFO.ElectrochemicalThermodynamicQuantity
- is_a emmo.ElectricPotential

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

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

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

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

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

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

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

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

Chapter 4

Appendix

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