

D7.2 – Initial Version of the Battery Ontology

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ABSTRACT

The Battery Interface Ontology (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 classes 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 it 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). Throughout the development of BattINFO, reference documentation will be automatically generated to reflect the most current state of the ontology. It is available under the link: <https://big-map.github.io/BattINFO/>.



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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 electrochemistry, battery cells and their interfaces 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 a EMMO domain ontology.

BattINFO and Battery Value Chain Ontology (BVCO)

While BattINFO focuses on the internal components and chemical processes, it is designed to interact with the Battery Value Chain Ontology (BVCO)¹, which is also based on EMMO. BVCO is dedicated to the higher-level process chains for material processing and manufacturing and is

¹ https://github.com/BIG-MAP/BVCO_Mirror



therefore complementary to the BattINFO. The basic definition of the battery as a system is also made there. The BVCO is being developed under the coordination of Fraunhofer ISC as part of both EU and national research projects.

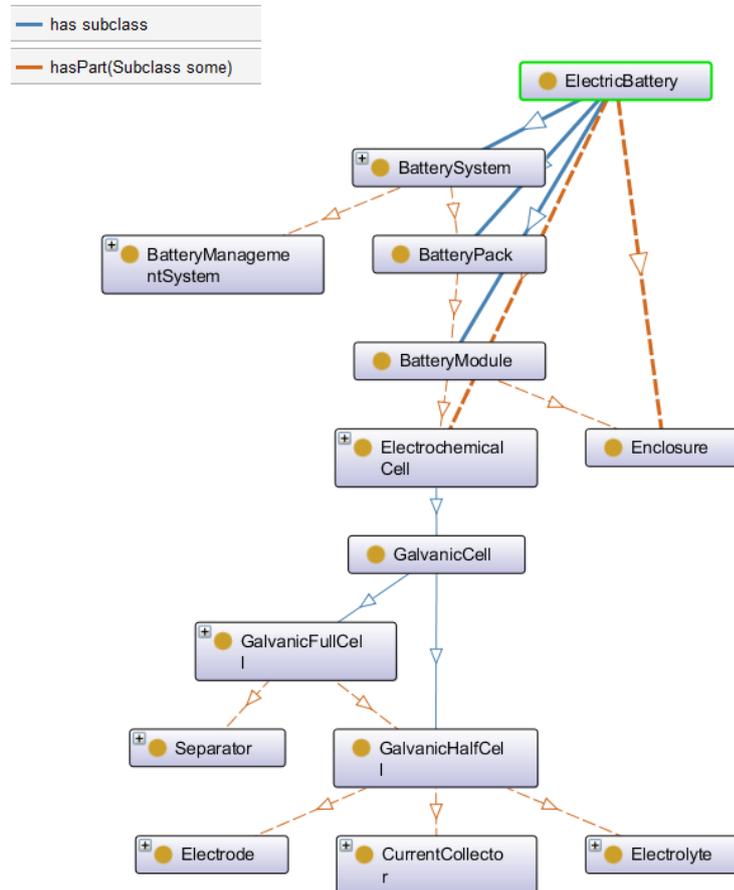


Figure 1. Overview of the (electric) battery definition in the BVCO

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

This report is structured as follows. In **Section 2 Battery Ontology Development**, the conceptual foundation for BattINFO is presented. This includes descriptions for the primary components in the battery ontology and justification for the design choices. In **Section 3 Implementation**, a description of the platform for collaborative development and implementation in the Ontology Web Language (OWL) is presented. In **Section 4 Summary and Outlook**, a summary of the work performed so far and an outlook towards the next steps in BattINFO development is provided.

BattINFO will continuously evolve over the course of the BIG-MAP project. Reference documentation for the most current version of the ontology is automatically generated and available under the link: <https://big-map.github.io/BattINFO/>.

2. Battery Ontology Development

This section presents the fundamental concepts that form the foundation for the ontology and the primary components that compose it. The concepts described here are the result of the first set of deliberations by the BattINFO working group.

BattINFO naming conventions adhere to the recommendations from EMMO. Classes are defined as nouns written in UpperCamelCase. In the figures of this report, the display names include spaces to make them practical to display and read.

Electrochemistry

EMMO is a diverse and well-developed top-level ontology for describing materials modelling and characterization. However, for the development of the BattINFO domain, it is helpful to propose some additional top-level concepts to describe common aspects of electrochemistry.

In EMMO, a quantitative property is defined as "a 'Quantity' that can be quantified with respect to a standardized reference physical instance (e.g. the prototype meter bar, the kg prototype) or method (e.g. resilience) through a measurement process." A quantitative property can be assigned either by measuring the value through some semiotic process (a `MeasuredQuantitativeProperty`) or associating the property by convention or assumption (a `ConventionalQuantitativeProperty`). In the initial version of BattINFO, the working rule was applied that a `ConventionalQuantitativeProperty` is some property that is essential to the function of the object and/or could be easily found in a specification. Conventional quantitative properties become measured quantitative properties when associated to a semiotic measurement process. Furthermore, we define two sub-categories of quantitative properties to describe common properties associated to electrochemistry: `ConventionalElectrochemicalProperty`, and `MeasuredElectrochemicalProperty`.

EMMO provides a subclass of processes for `PhysicalPhenomenon`, which is defined as a process that is recognized by physical sciences and is categorized accordingly. BattINFO provides an analogous subclass `ChemicalPhenomenon` to describe a chemical process and `ElectrochemicalPhenomenon` to describe a chemical phenomenon that is accompanied by the flow of electric current.

A battery ontology must include some description of chemical and electrochemical reactions. In BattINFO, a `ChemicalReaction` class is created and categorized as a `ChemicalPhenomenon` with the description, "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')." [6]. Likewise, an `ElectrochemicalReaction` class is created and categorized as an `ElectrochemicalPhenomenon` with the definition, "Any process either caused or accompanied by the passage of an electric current and involving in most cases the transfer of electrons between two substances." In addition to the classes described above, BattINFO defines classes describing other foundational concepts in electrochemistry, including `CompositeReaction`, `ElementaryReaction`, `Oxidizing Agent`, `Product`, `RateDeterminingStep`, `Reactant`, `RedoxReaction`, `ReducingAgent`, and `StoichiometricEquation`. Please refer to the glossary for a complete list with definitions.



Finally, to facilitate the description of electrochemical cells and their respective components and materials, a chain of proposed electrochemical classes linked by spatial parthood are proposed in BattINFO including an `ElectrochemicalSystem`, `ElectrochemicalCell`, `ElectrochemicalComponent`, `ElectrochemicalSubcomponent`, and `ElectrochemicalMaterial` are defined and presented in Figure 1.

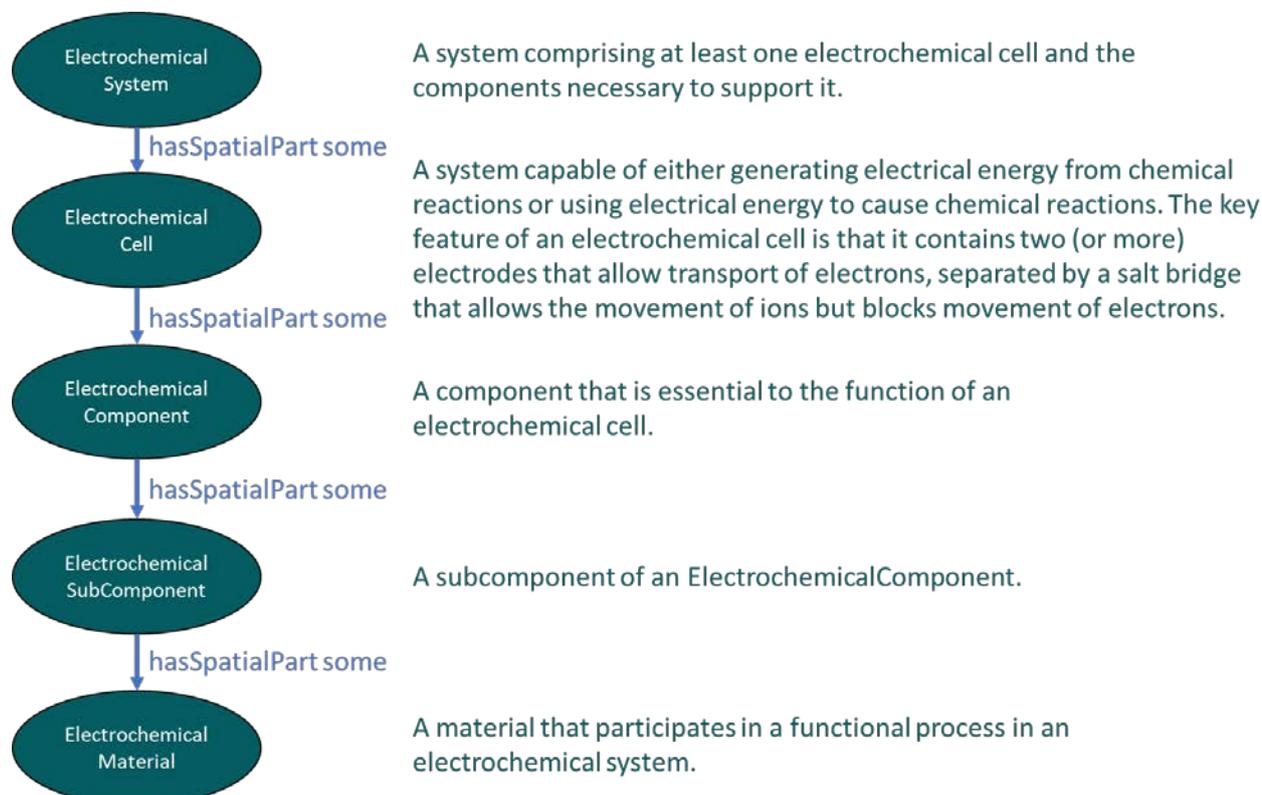


Figure 2. Chain of parthood and elucidations for some classes proposed in BattINFO.

Electrochemical Cell

Figure 3 provides an overview of the electrochemical cell taxonomy. IUPAC recommendations for terminology of electrochemical methods of analysis define an electrochemical cell as a, "system that consists of at least two electron conductors (electrodes) in contact with ionic conductors (electrolytes)" [7]. The two electrodes are often referred to as the Anode (i.e. electrode of an electrochemical cell through which net electric current flows and at which the predominating electrochemical reaction is an oxidation) and Cathode (i.e. electrode of an electrochemical cell through which net electric current flows and at which the predominating electrochemical reaction is a reduction). Although an electrochemical cell will have both an anode and a cathode, the respective electrodes that perform the oxidation or reduction reactions can change depending on if the battery is in a discharging or charging process. BattINFO addresses this by referring to electrodes by their relative polarity (positive and negative) rather than by anode or cathode, which are considered to be temporal parts (more in the Electrode Section, p. 8).

The role of the ionic conductor in the electrochemical cell is two-fold. It must conduct ions (but not electrons) between the electrodes and must physically separate the two electrodes to prevent an internal short-circuit. In BattINFO, this is achieved through a component called a salt bridge, defined



by IUPAC as a "means of making electrolytic connection between two half cells without introducing a significant liquid junction potential" [7] (more in the Salt Bridge Section, p. 12).

Electrochemical cells may be galvanic or electrolytic. A galvanic cell is an electrochemical cell in which chemical reactions occur spontaneously and chemical energy is converted into electrical energy. An electrolytic cell is an electrochemical cell in which electrical energy is converted into chemical energy. In battery jargon, a primary cell is a battery that is only discharged once and would be a galvanic cell. On the other hand, a secondary battery can be both discharged and recharged. In this case, it is a galvanic cell during the discharging process and an electrolytic cell during the charging process.

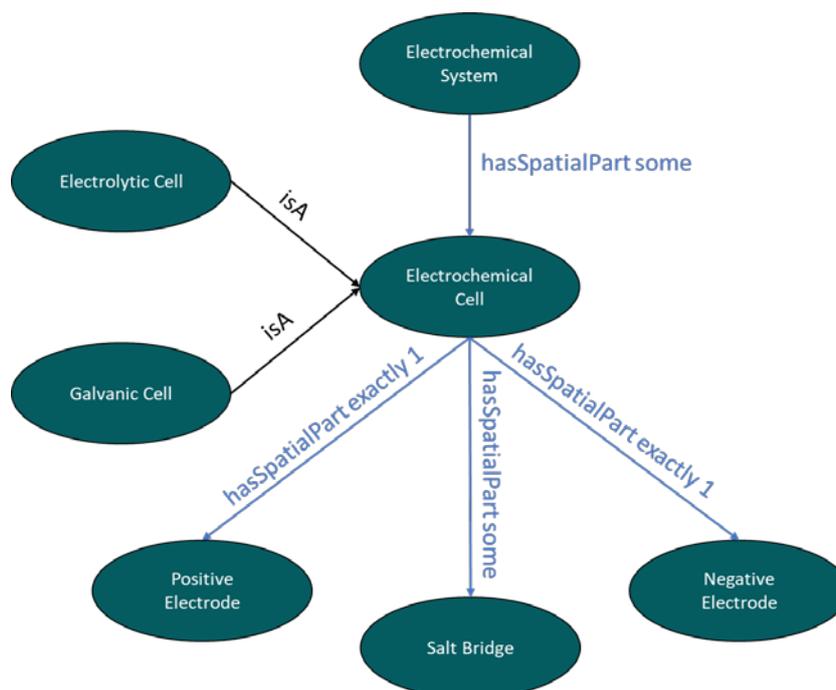


Figure 3. Overview of the ElectrochemicalCell taxonomy.

In the following sections, more detail is provided for the electrode and salt bridge branches.

Electrode

Figure 4 provides an overview of the basic relations for an electrode in BattINFO. An electrode is defined by IUPAC as, " 1. Electron conductor in an electrochemical cell connected to the external circuit. 2. Half-cell consisting of at least one electron conductor and at least one ionic conductor (electrolyte)." An electrochemical cell must contain at least two electrodes, which BattINFO distinguishes using the terms PositiveElectrode and NegativeElectrode. The positive electrode is identified as the electrode with the lowest electrochemical potential, and the negative electrode is identified as the electrode with the highest electrochemical potential.

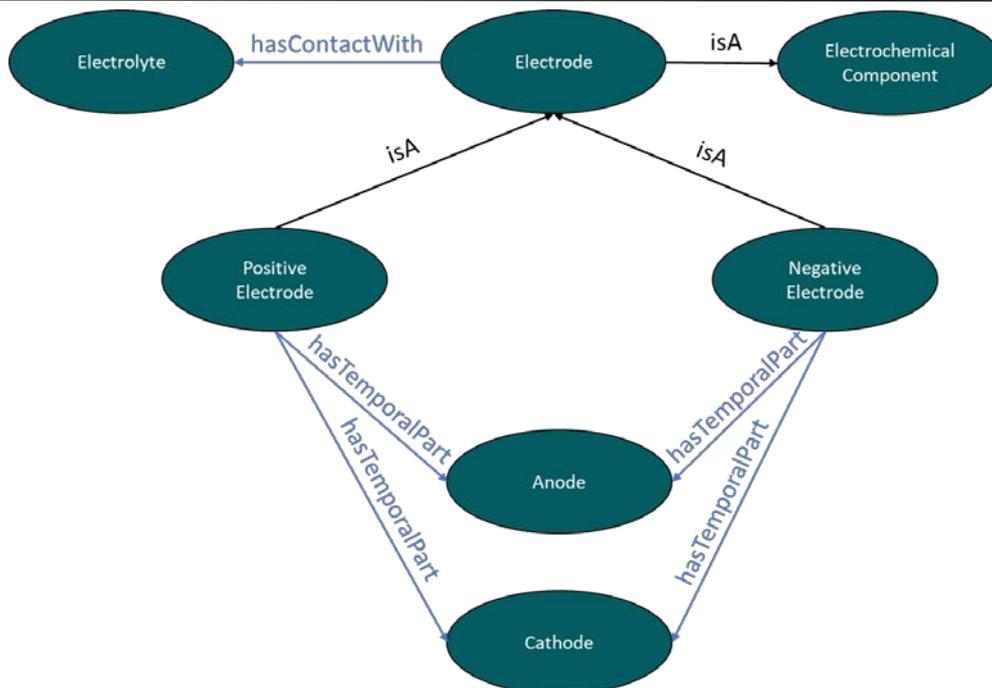


Figure 4. Overview of the relationships between PositiveElectrode, NegativeElectrode, Anode, and Cathode.

Electrodes can take a variety of forms. An electrode may be as simple as a metal foil or wire, which is structurally stable and acts as both the material which surface is electrochemically active and current collector. Most real electrodes are more complex. For example, Li-ion batteries use composite electrodes featuring a paste of electrochemically active material particles –direct participants in the dominant electrochemical reaction- and electronically conductive additives held together by a polymer binder and coated onto a metal foil current collector. Gas diffusion electrodes in metal-air batteries are based on some electronically conductive porous substrate loaded with an electrocatalyst and treated with PTFE to create a three-phase boundary between the gas, electrolyte, and catalyst. Such examples of composite electrodes comprise a variety of constituents that are designed with a primary role in mind. In BattINFO, roles considered for electrode constituents are electrochemical, structural, and electronic. The electrode's relationships to its constituents are outlined in Figure 5.

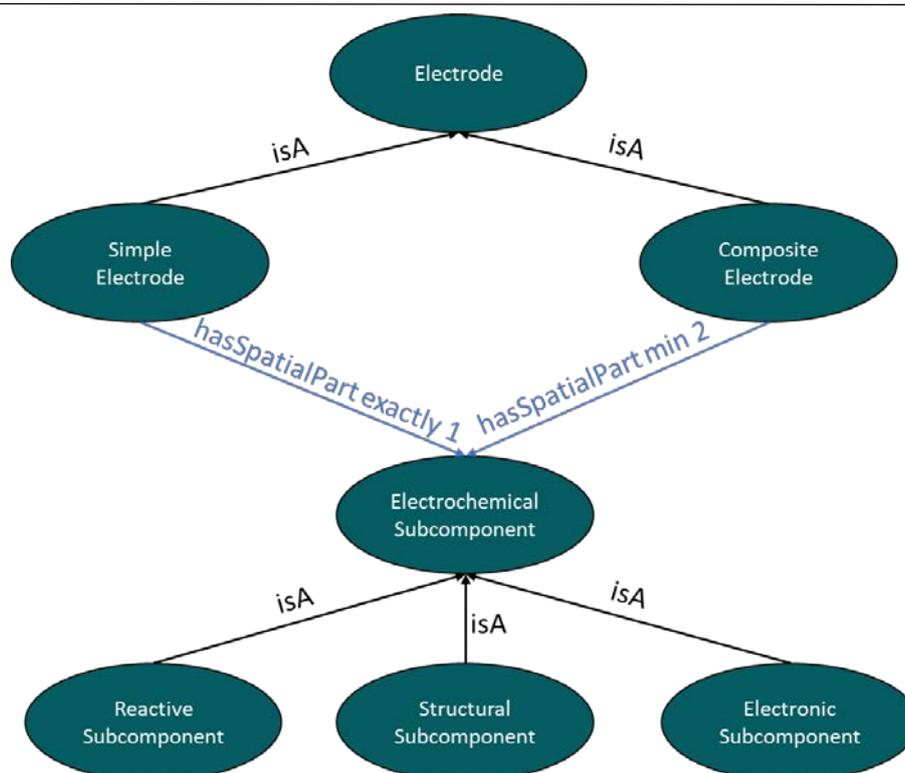


Figure 5. Overview of the relations between a SimpleElectrode and a CompositeElectrode.

Figure 6 shows some examples of electrochemical, structural, and electronic electrode constituents. Electrochemical constituents are defined as a constituent whose primary role is electrochemical. This may include materials like electrocatalysts that facilitate the electrochemical reaction but do not participate themselves or battery active materials that participate directly in the electrochemical reactions.

An electroactive substance is defined by IUPAC as a substance that undergoes a change of oxidation state, or whose chemical bonds are broken or formed in a charge-transfer reaction at an electrode [7]. An electrode active material is a material containing an electroactive substance that is a spatial part of the electrode domain. For example, in Li-ion batteries, C_6 and LiC_6 are electrode active materials because they are a spatial part of the electrode, but Li^+ is not (even though it is an electroactive substance).

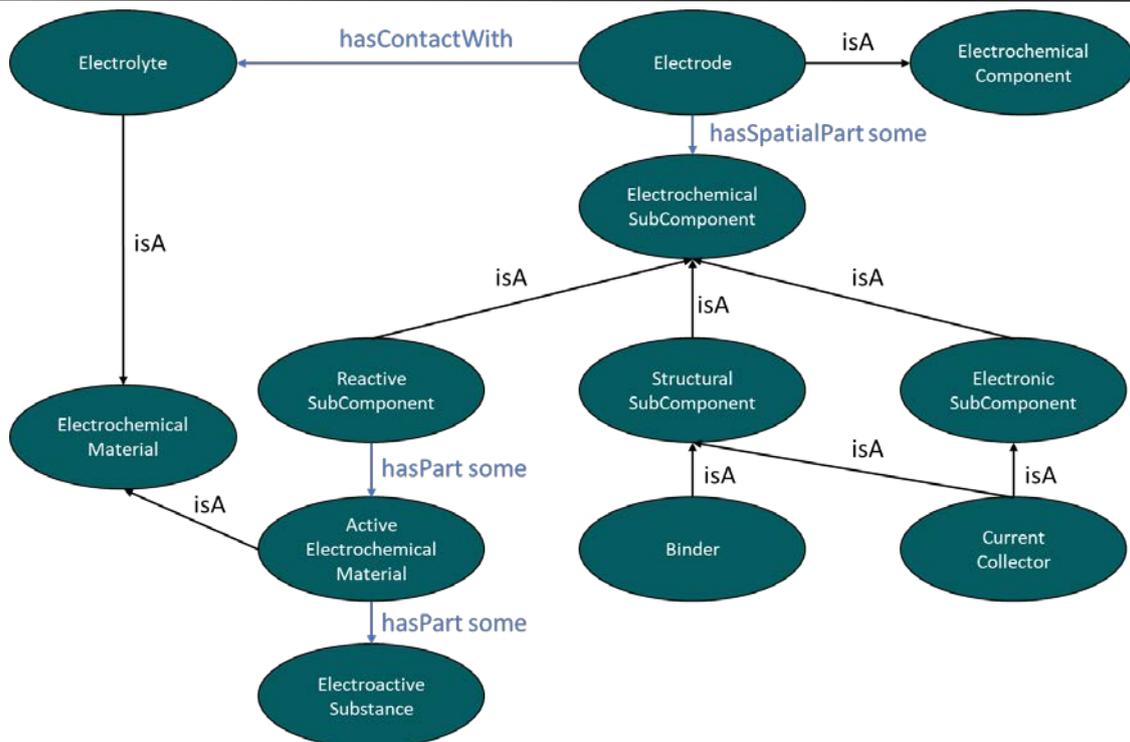


Figure 6. Overview of the relations between Electrode and ElectrochemicalSubComponents.

An example of a structural constituent is a binder, often a polymer like PTFE, which is included to improve the structural stability of a composite electrode. Some constituents can span categories, for example the current collector, which is both an electronic constituent (as its main purpose is to conduct electrons to/from the electrode) and a structural constituent (as by nature of its continuous conducting matrix it inherently provides additional structural stability).

Finally, one important class of electrode to consider in a battery ontology is the porous electrode. Electrochemical Systems [1] defines a porous electrode as:

"an electrode that consists 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."

For the purpose of the description in BattINFO, we define a PorousElectrode as having a spatial part ElectrodePore that itself has a spatial part Electrolyte.

From both the fundamental definition of the electrode and its most widely used sub-class the porous electrode, it is clear that the electrode electrolyte interface is an important part of battery performance. This will be more deeply explored in future versions of BattINFO. For the moment, we will concentrate on the other component in which the electrolyte plays a deciding role, the salt bridge.

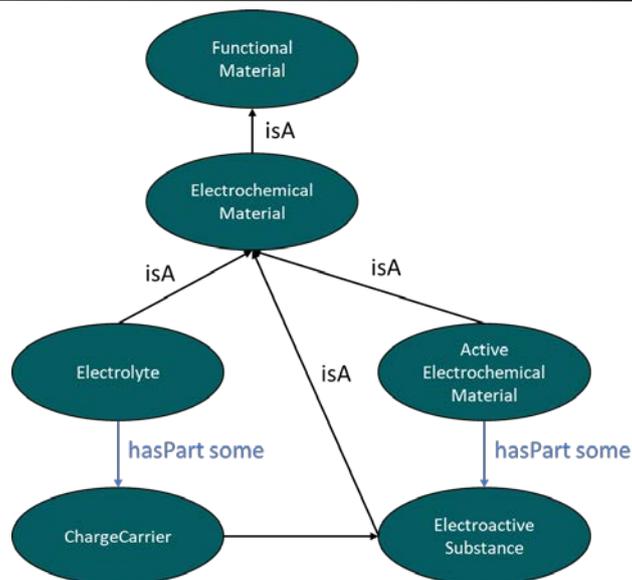


Figure 7. Overview of ElectrochemicalMaterial relations.

Salt Bridge

IUPAC defines a salt bridge as a means of making electrolytic connection between two half cells without introducing a significant liquid junction potential [7]. As with the electrolyte, BattINFO allows for the description of a simple salt bridge (consisting of a single constituent) or a composite salt bridge (consisting of two or more constituents), shown in Figure 8. Constituents in the salt bridge can fulfil two roles: structural and ionic transport.

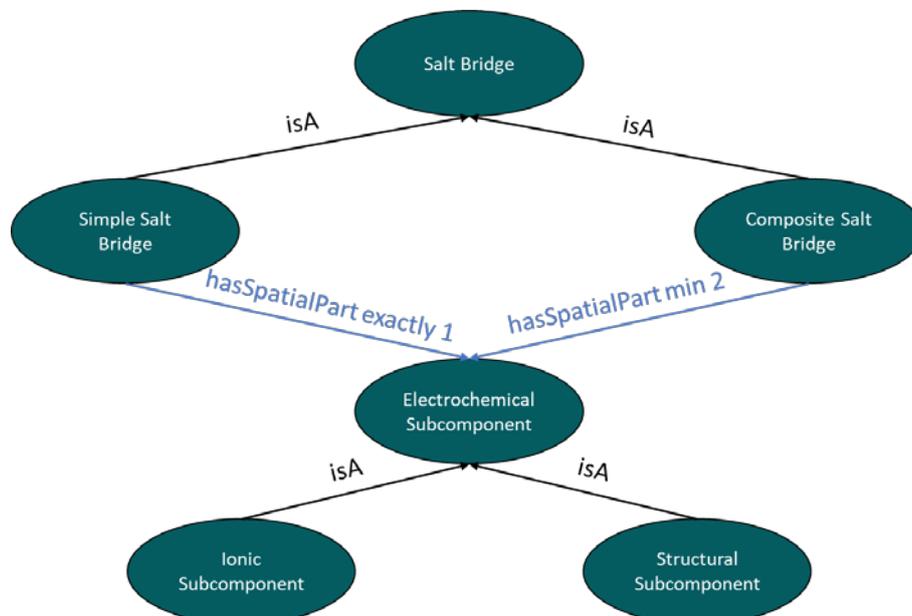


Figure 8. Overview of the relations in the SaltBridge branch.

A structural constituent is intended to provide some structural integrity to the salt bridge. The ionic transport constituent is designed to facilitate the transport of ions between the electrode. The classical design of a composite salt bridge features structural components that are the tube and porous stoppers and ionic transport constituent that is the supporting electrolyte. In Li-ion batteries today, the structural constituent is the porous separator and the ionic transport constituent is the



electrolyte. In laboratory cells in which the electrodes are separated only by an electrolyte bath, then the salt bridge is a simple salt bridge with the single constituent of the electrolyte as an ionic transport constituent.

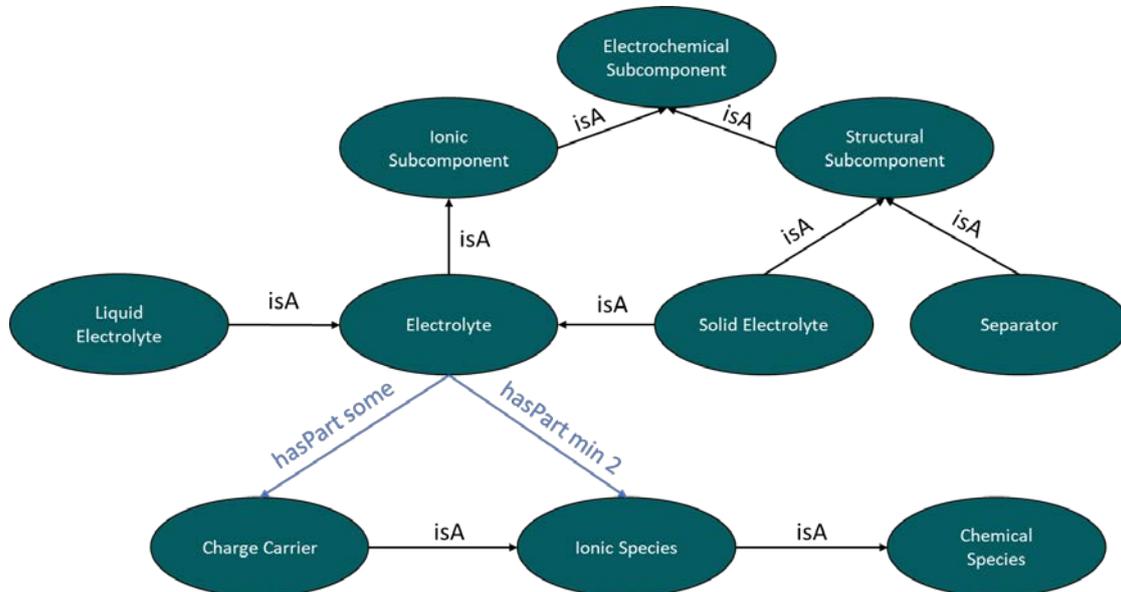


Figure 9. Overview of Electrolyte relations.

As with the electrode, some constituents can span multiple classes, as shown in Figure 9. For example, a solid electrolyte is both a structural constituent (as it provides structural integrity to the salt bridge) and an ionic constituent as it is an electrolyte.

An electrolyte is defined by IUPAC [7] as:

1. Conducting medium in which the flow of electric current is accompanied by the movement of ions.
2. Substance that provides ions on dissolution in a solvent or on melting.

An electrolyte must have some mobile ion, known in battery jargon as the charge carrier. To maintain electroneutrality, the charge carrier must be balanced by a second ionic species of opposite charge. In liquid electrolytes, this is achieved by a so-called counterion. In solid electrolytes, it is achieved by the fixed charge groups.

There are two common liquid electrolytes currently in use for battery applications: electrolytic solutions and ionic liquids, as shown in Figure 10.

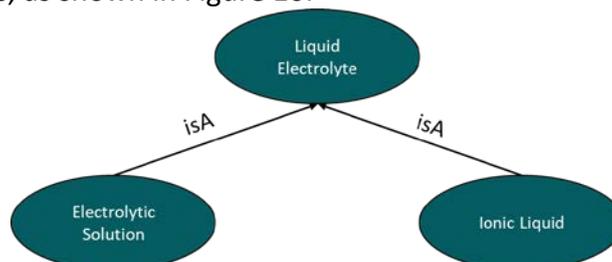


Figure 10. Overview of LiquidElectrolyte relations.



Figure 11 provides an overview of the relations for an electrolytic solution. Electrolytic solutions are liquid electrolytes that contain a solvent and solutes. In electrochemical applications, electrolytic solutions are often either aqueous solutions (using water as a solvent) or organic solutions (using an organic molecule as a solvent, e.g. ethylene carbonate).

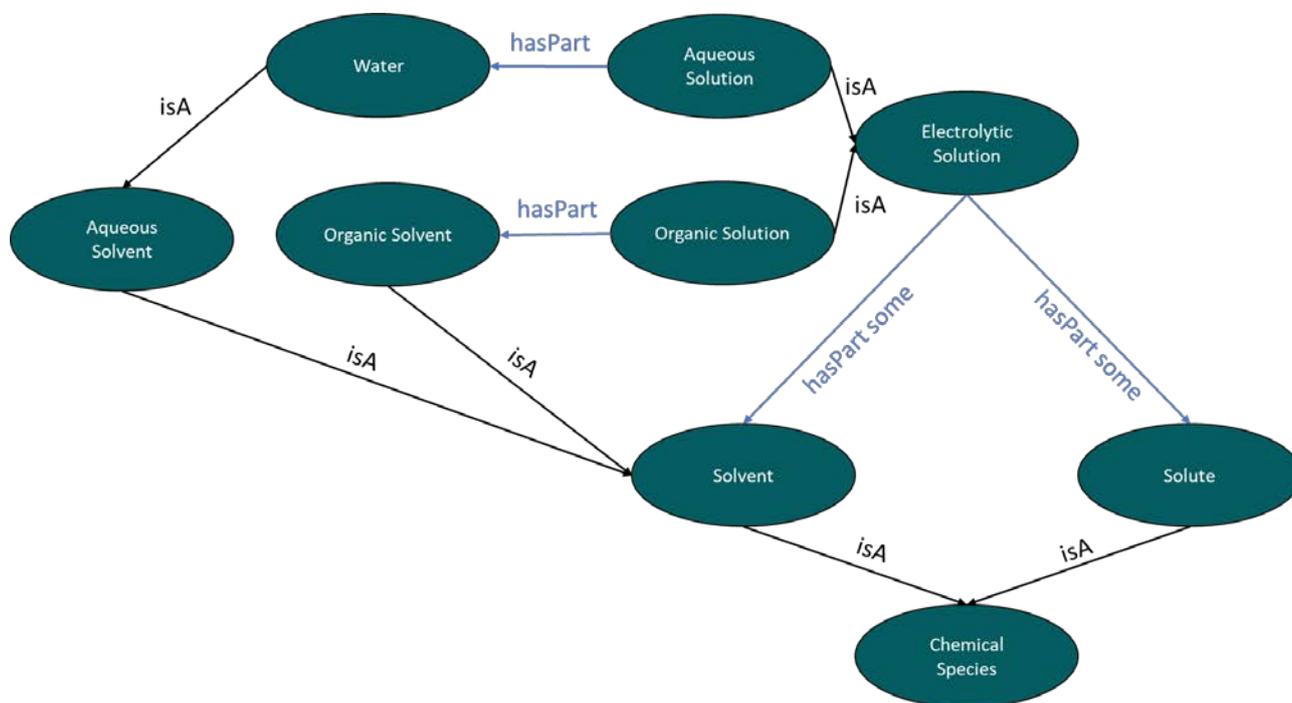


Figure 11. Overview of ElectrolyticSolution relations.

Observations

In EMMO, the definition of class properties is associated to the observation procedure that is used to measure the quantity. To accomplish this, the measurement is described as a semiotic process in which an 'interpreter' is used to create a 'sign' that describes some 'object'. The definition of observation processes (Figure 12) is also necessary to support BIG-MAP project activities such as the establishment of the online lab notebook. Semiotic processes defined in BattINFO should overlap with definitions in the online lab notebook to facilitate the seamless integration of data into the ontology.

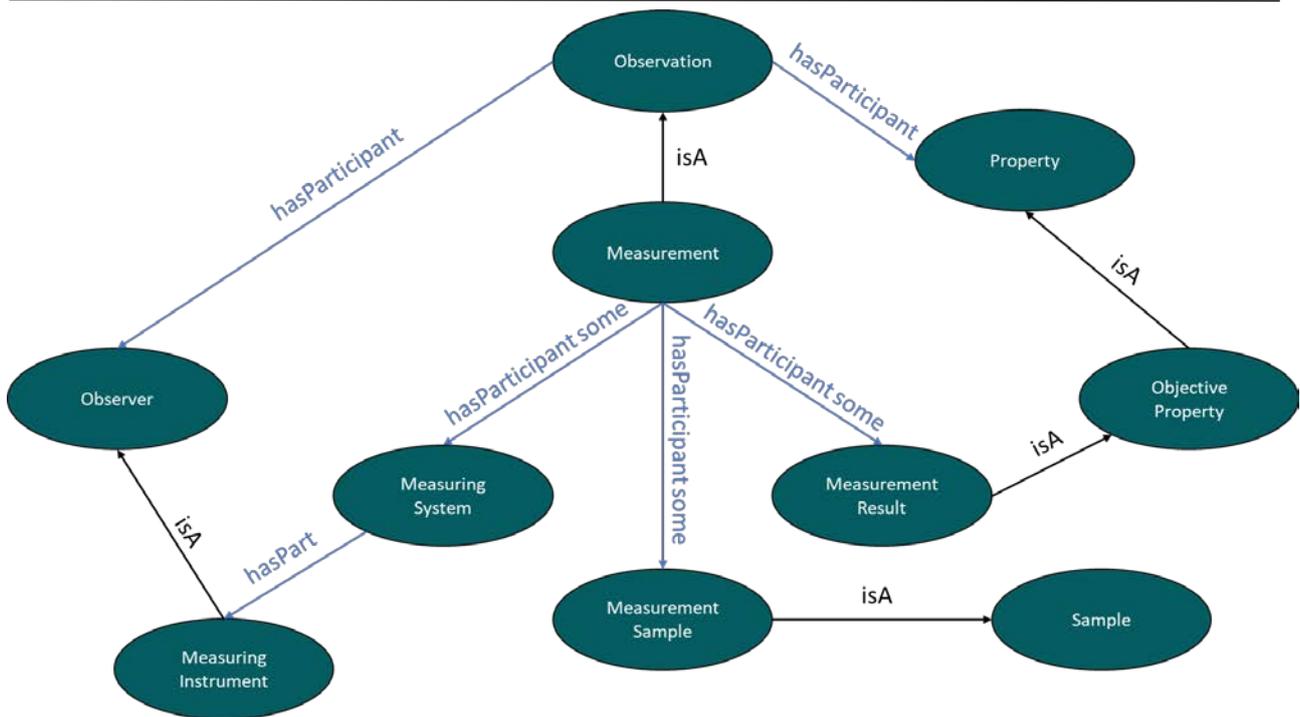


Figure 12. Overview of the relations in an Observation.

There are many observation processes that are part of characterizing the properties of batteries and their interfaces. These will be constantly added and refined in the ontology throughout the BIG-MAP project. As a starting point, we consider a common measurement process: diffraction.

An overview of the relations in a diffraction measurement process is shown in Figure 13. A diffraction measurement has participants diffraction measuring system, sample, and diffraction measurement result. A diffraction measurement system has parts for measuring instruments diffraction instrument and software.

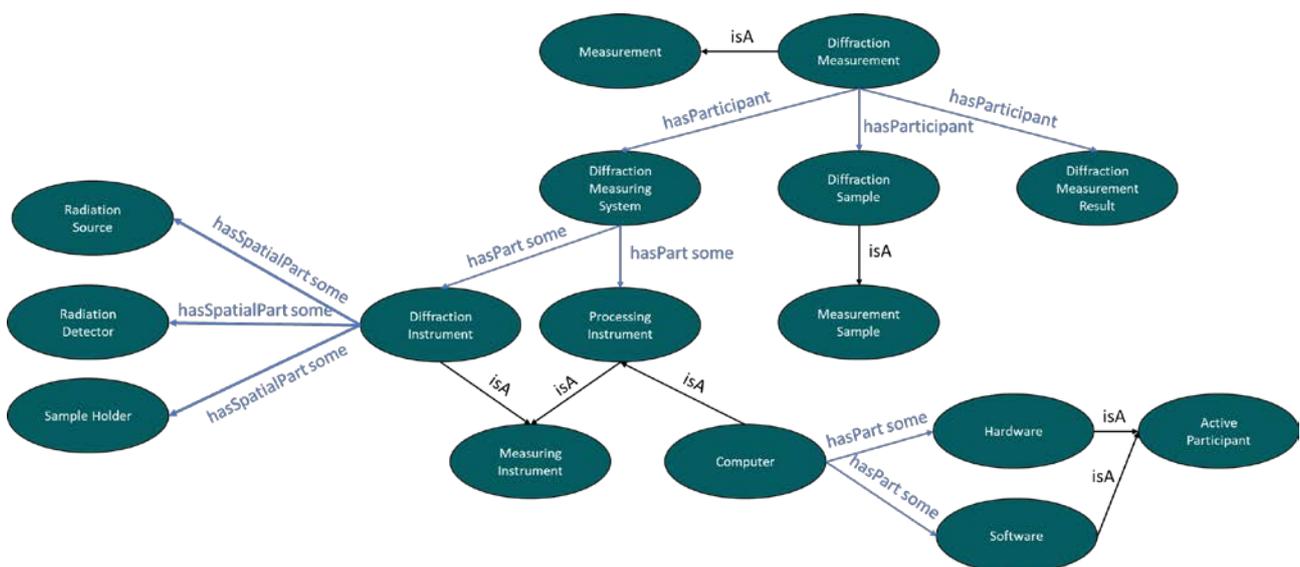
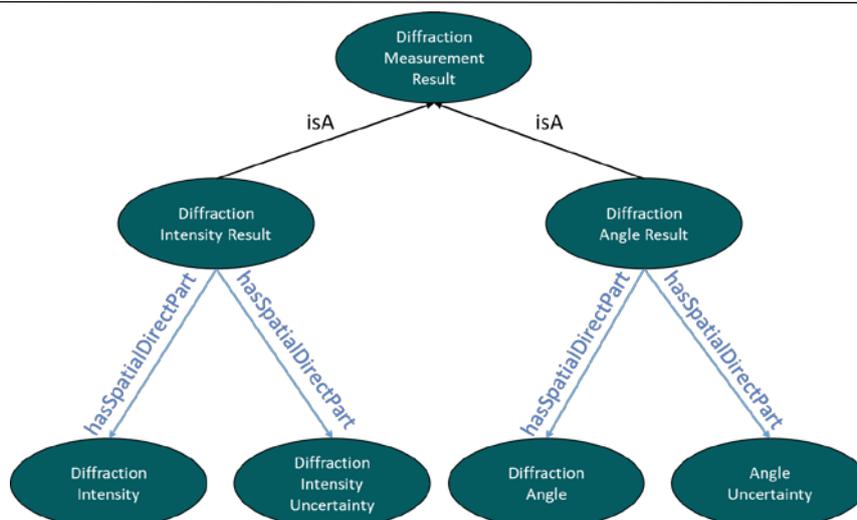


Figure 13. Overview of DiffractionMeasurement relations.



The diffraction measurement result is composed of two quantities, count vector and angle vector, which are participants in a LeBail fitting process to extract the objective property lattice parameter, as shown in Figure 14.

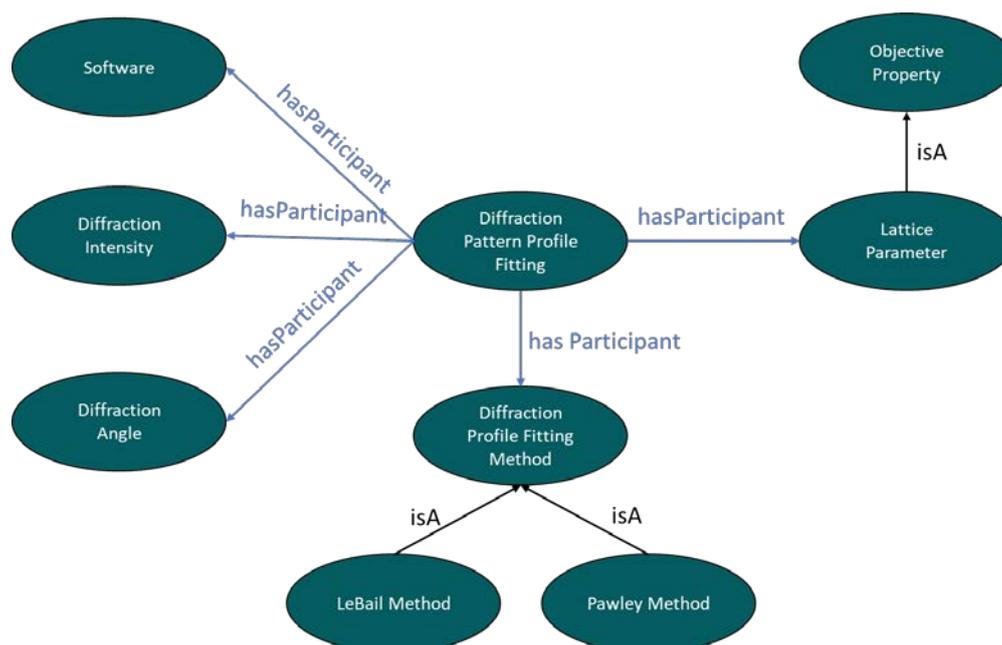


Figure 14. Overview of relations for extracting lattice parameters from a diffraction measurement result.

Equations and Models

In BattINFO, equations give context to the relationships between properties and are the foundational components of models. There are many equations that describe electrochemical phenomena which could be used to characterize batteries and their interfaces. These will be consistently added and refined in the ontology during the BIG-MAP project. As a starting point, we have included annotations for some foundational equations and shown how they may be incorporated into a model.



The Butler-Volmer equation is the standard phenomenological model for electrode kinetics. It fits the current-voltage characteristic of many electrodes and can be partially justified by Marcus theory of charge-transfer reaction kinetics. The equation takes the form:

$$i = i_0 \left\{ \exp \left[\frac{\alpha_a n F}{RT} \eta_S \right] - \exp \left[- \frac{\alpha_c n F}{RT} \eta_S \right] \right\}. \quad (1)$$

where i is the electrode current, i_0 is the exchange current, α_a is the anodic charge transfer coefficient, α_c is the cathodic charge transfer coefficient, n is the electron number, F is the Faraday constant, and η_S is the surface overpotential. The surface overpotential is defined as:

$$\eta_S = \Phi_{\text{elde}} - \Phi_{\text{elyte}} - E^{\text{eq}}. \quad (2)$$

In the annotation of the equation, given in Table 1, the quantities that are involved in the equation are considered spatial direct parts of the equation.

Table 1. Annotation for the Butler-Volmer equation.

ButlerVolmerEquation
<i>The standard phenomenological model for electrode kinetics. $i = i_0 * (\exp(\alpha * n * F * \eta / (R * T)) - \exp(-(1 - \alpha) * n * F * \eta / (R * T)))$.</i>
isA ElectrochemicalEquation
<i>hasSpatialDirectPart</i> Current
<i>hasSpatialDirectPart</i> ExchangeCurrent
<i>hasSpatialDirectPart</i> SurfaceOverpotential
<i>hasSpatialDirectPart</i> ChargeTransferCoefficient
<i>hasSpatialDirectPart</i> ElectronNumber
<i>hasSpatialDirectPart</i> FaradayConstant
<i>hasSpatialDirectPart</i> MolarGasConstant
<i>hasSpatialDirectPart</i> ThermodynamicTemperature

The Nernst equation is a fundamental equation in electrochemistry that describes the dependence of the equilibrium electrode potential on the composition of the contacting phases. It is an expression of thermodynamic equilibrium derived from the law of mass action:

$$E^{\text{eq}} = E^0 - \frac{RT}{nF} \ln(Q). \quad (3)$$

where E^{eq} is the equilibrium electrode potential, E^0 is the standard electrode potential, and Q is the reaction quotient. The annotation for the Nernst equation is given in Table 2.

Table 2. Annotation for the Nernst equation.

NernstEquation
<i>Fundamental equation in electrochemistry that describes the dependence of the equilibrium electrode potential on the composition of the contacting phases, written as a reduction: $E_{\text{eq}} = E^0 - (R * T / (z * F)) * \ln(Q)$. where E_{eq} is the equilibrium electrode potential, E^0 the standard electrode potential of</i>



the reaction, R the gas constant, T the thermodynamic temperature, F the Faraday constant, z the electron number of the electrochemical reaction, and ν_i are the stoichiometric coefficients (numbers of species) in the equation of the electrode reaction, positive for products and negative for reactants, while a_i represents the activities of the species involved (most usually ions).

isA ElectrochemicalEquation

hasSpatialDirectPart **EquilibriumElectrodePotential**
hasSpatialDirectPart **StandardElectrodePotential**
hasSpatialDirectPart **MolarGasConstant**
hasSpatialDirectPart **ThermodynamicTemperature**
hasSpatialDirectPart **ElectronNumber**
hasSpatialDirectPart **FaradayConstant**
hasSpatialDirectPart **ReactionQuotient**

The Nernst-Planck equation is a conservation of mass equation used to describe the motion of a charged chemical species in a fluid medium.

$$\frac{\partial c}{\partial t} = -\nabla \cdot \left(-D \left[\nabla c + \frac{zF}{RT} c(\nabla \phi) \right] \right). \quad (4)$$

The Nernst-Planck equation is valid in dilute solutions in which the effects of ion-ion interactions are negligible. The annotation for the Nernst-Planck equation is given in Table 3.

Table 3. Annotation for the Nernst-Planck equation.

NernstPlanckEquation
<i>A conservation of mass equation used to describe the motion of a charged chemical species in a fluid medium.</i>
isA PhysicsEquation
<i>hasSpatialDirectPart</i> Concentration <i>hasSpatialDirectPart</i> DiffusionCoefficient <i>hasSpatialDirectPart</i> IonicValence <i>hasSpatialDirectPart</i> ThermodynamicTemperature <i>hasSpatialDirectPart</i> FaradayConstant <i>hasSpatialDirectPart</i> ElectricPotential

The Nernst-Einstein equation relates the limiting molar conductivity of an electrolyte to the ionic diffusion coefficients of its constituents:

$$\Lambda_m^0 = \left(\frac{F^2}{RT} \right) (\nu_+ z_+^2 D_+ + \nu_- z_-^2 D_-). \quad (5)$$

where Λ_m^0 is the limiting molar conductivity, ν is the number of cations/anions per formula unit of electrolyte, z is the charge number, and D is the diffusion coefficient. The annotation for the Nernst-Einstein equation is given in Table 4.

Table 4. Annotation for the Nernst-Einstein equation.

NernstEinsteinEquation
<i>An equation relating the limiting molar conductivity to the ionic diffusion coefficients</i>



BIG-MAP



isA MaterialRelation

hasSpatialDirectPart **LimitingMolarConductivity**
hasSpatialDirectPart **FaradayConstant**
hasSpatialDirectPart **MolarGasConstant**
hasSpatialDirectPart **ThermodynamicTemperature**
hasSpatialDirectPart **IonsPerElectrolyte**
hasSpatialDirectPart **IonicValence**
hasSpatialDirectPart **DiffusionCoefficient**

3. Implementation

The Battery Interface Ontology (BattINFO) code repository is hosted on the collaborative coding and dissemination platform GitHub at www.github.com/BIG-MAP/BattINFO. A screenshot of the repository homepage is shown in Figure 15. The ontology is implemented in the ontology web language (OWL) and can be accessed and edited through the free ontology editor Protégé².

The screenshot displays the GitHub repository page for 'BIG-MAP / BattINFO'. At the top, there is a search bar and navigation links for Pull requests, Issues, Marketplace, and Explore. Below the repository name, there are statistics for Watch (2), Star (0), and Fork (0). The main navigation bar includes Code, Issues (4), Pull requests (1), Actions, Projects (1), Wiki, Security, Insights, and Settings. The file browser shows a list of files and folders, with the most recent commit being 'WIP: Added first entries to saltbridge (#34)' 3 days ago. The file 'battery.ttl' is highlighted. On the right side, there are sections for About (describing the ontology as based on EMMO), Releases (no releases published), Packages (no packages published), and Contributors (4 contributors listed: francescalb, jesper-friis, CasperWA, and jsimonclark).

Figure 15. Screenshot of the BattINFO repository on GitHub.

² <https://protege.stanford.edu/>



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Continuous Integration is ensured with Github-actions. For each change pushed to the repository an environment is built on which testing of the BattINFO ontology is done with respect to EMMO standards with the tool emmocheck from EMMO-python.

For the sake of development the BattINFO is structured with a top ontology `battinfo.ttl` that imports ontologies of the various sub-domains according to Figure 16. `Battinfo.ttl` imports the files `observations.ttl` and `models.ttl` that describe observation processes and models, respectively. These files import `battery.ttl` which describe the overall battery. The main components, electrode and saltbridge are then included as separate subontologies. Battery specific properties import the more general electrochemical properties. Finally EMMO is imported. In between, `generic-properties` is imported, which contains properties to be included in the main EMMO at a later stage. This is done to make it easy to define concepts that we think would naturally belong to EMMO without introducing delays in the development of BattINFO when waiting for our proposed contributions to be accepted.

The namespace of BattINFO is '`http://emmo.info/BattINFO`', as the intention is to propose BattINFO as a domain ontology within the EMMC umbrella. The entities described in '`generic-properties`' are given the EMMO namespace '`http://emmo.info/emmo`' for easier inclusion into EMMO itself.

BattINFO is implemented using the turtle file format, adopting the format currently used by EMMO. The choice of file format has no effect on semantics and the choice of changing from `rdf/xml` (`.owl` suffix) to the more readable turtle (`.ttl`) format is purely practical.

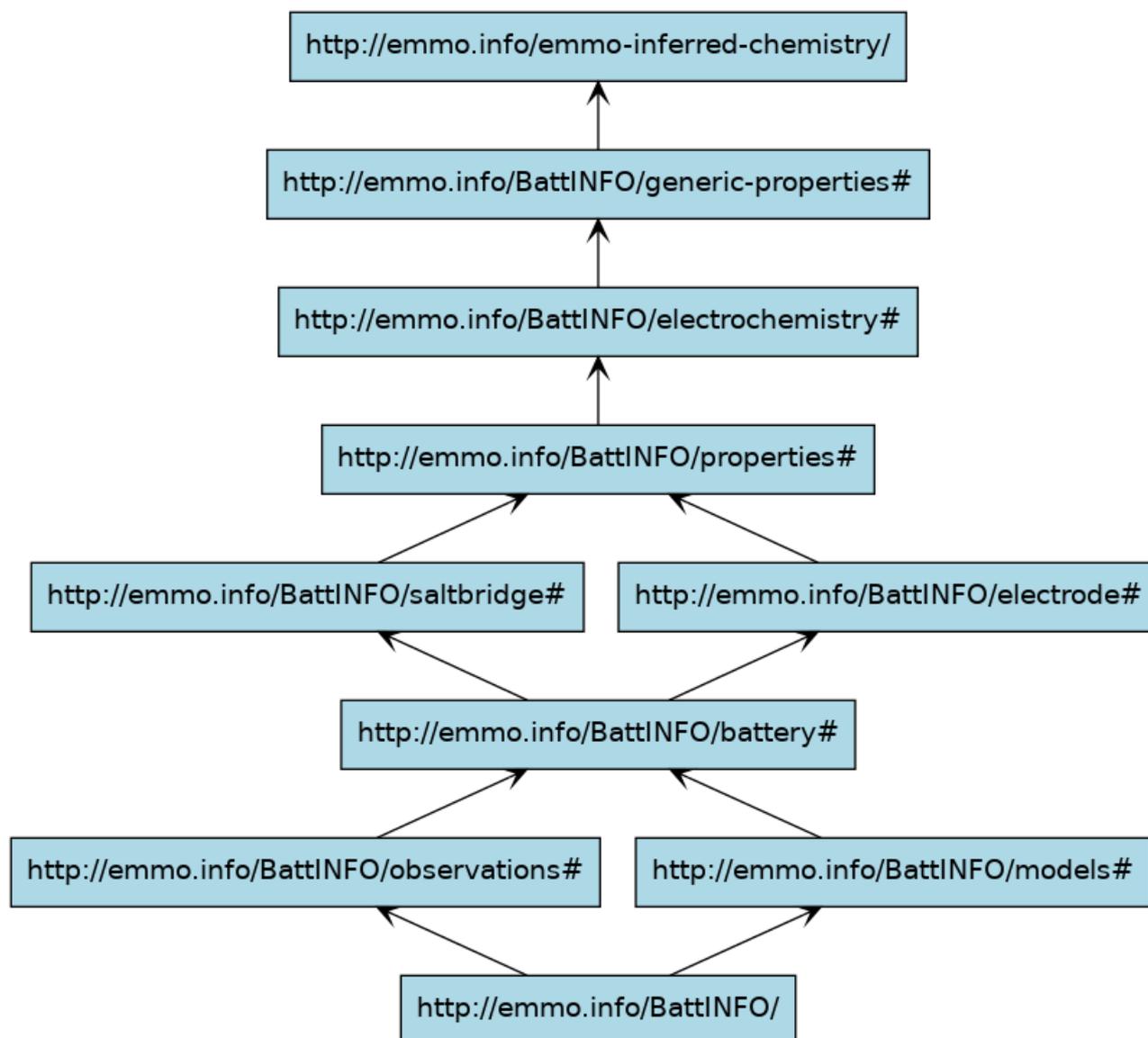


Figure 16. The structure of BattINFO. This is subject to change and simplification when the ontology is more mature.

4. Summary and Outlook

This report presents the conceptual basis for the first version of the BIG-MAP Battery Interface Ontology (BattINFO). BattINFO is an ontology of batteries and their interfaces based on the top-level European Materials and Modelling Ontology (EMMO)³. The electrochemical concepts and definitions included in BattINFO are based as far as possible on accepted standards from the International Union of Pure and Applied Chemistry (IUPAC) [6], [7] or other preeminent textbooks on the subject such as Electrochemical Systems [1].

³ <https://www.emmo.info/>



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The initial version of BattINFO includes descriptions of fundamental concepts in electrochemistry, electrochemical cells, electrodes, salt bridge, observations, equations, and models. The definitions of classes 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.

Glossary

The glossary in Table 5 contains a list of classes defined in BattINFO with their descriptions.

Table 5. Glossary of major classes in BattINFO.

OBJECT	ELUCIDATION
Acid	"A molecular entity or chemical species capable of donating a hydron (proton) (see Brønsted acid) or capable of forming a covalent bond with an electron pair (see Lewis acid)." [6]
ActiveElectrochemicalMaterial	a material containing an electroactive substance that is a spatial part of the electrode domain
ActiveParticipant	A 'physical' that stands for a real-world object that takes active part of a functional process.
Anion	"A monoatomic or polyatomic species having one or more elementary charges of the electron." [6]
Base	"A chemical species or molecular entity having an available pair of electrons capable of forming a covalent bond with a hydron (proton) (see Brønsted base) or with the vacant orbital of some other species (see Lewis base)." [6]
BulterVolmerEquation	"The standard phenomenological model for electrode kinetics"
Cation	"A monoatomic or polyatomic species having one or more elementary charges of the proton." [6]
ChemicalPhenomenon	"A 'process' that is recognized by chemical sciences and is categorized accordingly."
ChemicalReaction	"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')." [6]
ChemicalSpecies	"Ions as well as molecular components that do not dissociate" [1]
CompositeReaction	"A chemical reaction for which the expression for the rate of disappearance of a reactant (or rate of appearance of a product) involves rate constants of more than a single elementary reaction." [6]
ConventionalElectrochemicalProperty	"A ConventionalQuantitativeProperty that is unique to the field of electrochemistry"
DiffractionInstrument	"An instrument that measures the diffraction of an electromagnetic wave (originating from a source) through a sample as seen by a detector."



DiffractionMeasurement	"A measurement of the wave diffraction property of some sample."
DiffractionMeasurementResult	"A result from a Diffraction Measurement."
DiffractionMeasuringSystem	"A system for measuring diffraction patterns and processing the result."
ElectrochemicalCell	<p>"System that consists of at least two electron conductors (electrodes) in contact with ionic conductors (electrolytes).</p> <p>Note 1: The two electrodes may be a working electrode and an auxiliary electrode or, for zero-current measurements (potentiometric mode), an indicator electrode and a reference electrode. There may be a third electrode, the cell having a separate auxiliary electrode (to carry current) and reference electrode (for measurement of electrode potential) in addition to a working electrode (See three-electrode cell).</p> <p>Note 2: The current flow through the electrochemical cell may be zero or non-zero. An electrochemical cell with current flow can operate either as a galvanic cell or as an electrolytic cell.</p> <p>Note 3: In electrochemistry the term "cell" is commonly qualified to describe the particular device on which electrochemical reactions take place. Examples of galvanic and electrolytic cells are standard cells, electrochemical sensor cells, conductivity cells, spectroelectrochemical cells, fuel cells, batteries, electrochemical measuring cells, and two- and three-electrode cells. Note 4: If processes of interest occur at both the anode and the cathode of a cell (as in differential amperometry or controlled-current potentiometric titration with two indicator electrodes), the cell should be said to comprise two indicator or two working electrodes." [7]</p>
ElectrochemicalComponent	"A component in an electrochemical device (electrode or salt bridge)."
ElectrochemicalContinuumModel	"A continuum model of an electrochemical cell coupling electrochemistry with mass, charge, and energy transport. The model is often discretized and solved using numerical methods including the finite difference method, finite volume method, or finite element method. The primary mesh is discretized through the transverse direction of the cell, with the secondary mesh along the radius of the active material particles."
ElectrochemicalDevice	A device whose primary function is facilitating the conversion between chemical and electrical energy.
ElectrochemicalEquation	"An equation that describes an electrochemical phenomenon."
ElectrochemicalMaterial	"A material synthesized in a manufacturing process for a specific use in an electrochemical device."
ElectrochemicalPhenomenon	"A chemical phenomenon that is accompanied by the flow of electric current."



ElectrochemicalReaction	"Any process either caused or accompanied by the passage of an electric current and involving in most cases the transfer of electrons between two substances"
ElectrochemicalSubcomponent	A subcomponent of an ElectrochemicalComponent.
ElectrochemicalSystem	A system comprising at least one electrochemical cell and the components necessary to support it.
Electrolyte	"1. Conducting medium in which the flow of electric current is accompanied by the movement of ions. 2. Substance that provides ions on dissolution in a solvent or on melting." [7]
ElectrolyticCell	"Electrochemical cell in which electrical energy is converted into chemical energy." [7]
ElectrolyticSolution	"A liquid electrolyte that consists of solutes dissolved in a solvent."
ElementaryReaction	"A reaction for which no reaction intermediates have been detected or need to be postulated in order to describe the chemical reaction on a molecular scale. An elementary reaction is assumed to occur in a single step and to pass through a single transition state." [6]
FicksFirstLaw	"Relates the diffusive flux to the gradient of the concentration. It postulates that the flux goes from regions of high concentration to regions of low concentration, with a magnitude that is proportional to the concentration gradient (spatial derivative)"
FicksSecondLaw	"Predicts how diffusion causes the concentration to change with respect to time."
FunctionalMaterial	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.
GalvanicCell	"Electrochemical cell in which chemical reactions occur spontaneously and chemical energy is converted into electrical energy." [7]
IonicLiquidElectrolyte	"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." [7]
IonicSpecies	"An atomic or molecular particle having a net electric charge."
KohlrauschsLaw	"The migration of an ion at infinite dilution is dependent on the nature of the solvent and on the potential gradient but not on the other ions present"



LawOfMassAction	"The rate of any chemical reaction is proportional to the product of the masses of the reacting substances, with each mass raised to a power equal to the coefficient that occurs in the chemical equation."
LeBailFitting	"a whole diffraction pattern profile fitting technique used to characterize the properties of crystalline materials"
LiquidElectrolyte	"An electrolyte in the liquid phase"
NernstEinsteinEquation	"An equation relating the limiting molar conductivity to the ionic diffusion coefficients"
NernstEquation	Fundamental equation in electrochemistry that describes the dependence of the equilibrium electrode potential on the composition of the contacting phases, written as a reduction: $E_{eq} = E^0 - (R \cdot T / (z \cdot F)) \cdot \ln(Q)$. where E_{eq} is the equilibrium electrode potential, E^0 the standard electrode potential of the reaction, R the gas constant, T the thermodynamic temperature, F the Faraday constant, z the electron number of the electrochemical reaction, and Q is the reaction quotient of the reaction. [7]
NernstPlanckEquation	"A conservation of mass equation used to describe the motion of a charged chemical species in a fluid medium."
OxidizingAgent	"An element or compound that accepts an electron from an electron donator (reducing agent) in a redox chemical reaction."
Product	"A substance that is formed during a chemical reaction." [6]
RateDeterminingStep	"A rate-controlling (rate-determining or rate-limiting) step in a reaction occurring by a composite reaction sequence is an elementary reaction the rate constant for which exerts a strong effect — stronger than that of any other rate constant — on the overall rate." [6]
Reactant	"A substance that is consumed in the course of a chemical reaction. It is sometimes known, especially in the older literature, as a reagent, but this term is better used in a more specialized sense as a test substance that is added to a system in order to bring about a reaction or to see whether a reaction occurs (e.g. an analytical reagent)." [6]
RedoxReaction	"a type of chemical reaction that involves a transfer of electrons between two species."
ReducingAgent	"An element or compound that loses (or "donates") an electron to an electron recipient (oxidizing agent) in a redox chemical reaction."
RietveldFitting	"A least squares approach to refine a theoretical line profile until it matches the measured profile"



Salt	"A chemical compound consisting of an assembly of cations and anions." [6]
SaltBridge	"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 containing an electrolyte with approximately equal ion mobilities of the cation and the anion (e.g., KNO ₃ , KCl), with the ends of the tube immersed in the electrolyte solution of the half cells." [7]
ScanningElectronMicrograph	"An image obtained from a scanning electron microscope (SEM)"
ScanningElectronMicroscope	"A type of electron microscope that produces images of a sample by scanning the surface with a focused beam of electrons."
ScanningElectronMicroscopeSystem	"A system for measuring scanning electron micrographs and processing the results."
Separator	"A permeable membrane placed between the positive and negative electrodes to keep them physically separated and prevent an internal short circuit."
SolidElectrolyte	"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 Na _{1+x} Zr ₂ P _{3-x} Si _x O ₁₂ , 0 < x < 3." [7]
StoichiometricEquation	"The symbolic representation of a chemical reaction in the form of symbols and formulae, wherein the reactant entities are given on the left-hand side and the product entities on the right-hand side" [6]
StrongAcid	An acid that completely dissociates in water.
StrongBase	"A base that completely dissociates in water."
SupportingElectrolyte	"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." [7]
ThreeElectrodeCell	"Electrochemical cell with a working electrode, reference electrode, and auxiliary electrode. Note 1: Electric current flows between the working and auxiliary electrodes. Electrode potential may be measured between the working and reference electrodes. Note 2: A potentiostat can be used to maintain a potential difference between the working and reference electrodes."
WeakAcid	"An acid that partially dissociates in water."
WeakBase	"A base that partially dissociates in water."



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