Experimental Battery Research

Abstract

The project proposed is to design, build, and deliver a system which accurately generates new chemical batteries. This combinatoric chemical reaction problem requires a distributed system to explore the search space. Deployment of multiple models each using deep machine learning techniques will train with both theoretical and experimental data. The parallel models will be used to simulate & predict observable laboratory measurements used by AI search agents optimizing over battery characteristics. Reserved known chemical batteries will be used to validate predictions in situ to ensure there is confidence in testing new experimental batteries.

Contents

1 Phase 1: Feasibility study. Completed.

1.1 Planning and background.

The construction of an accurate simulation environment which can predict half-cell potentials, activation energies, and characterize battery performance before testing in the laboratory can reduce the costs of empirical testing by magnitudes. The disconnect between chemical composition, expected reaction physical configuration, and empirical measurements can be bridged using a series of AI and machine learning techniques to learn the real world results to build better approximate models. The databases of know material compounds is growing by inference the hyper graph of all possible reactions of those compounds is growing at an exponential rate. The perfect model for any equation is computationally expensive; there are some models which must operate with $> 99.99\%$ correctness, such as the mass laws of equation balancing. Fundamentally there are multiple models at varying scales that describe chemistry from approximately to exactly. Modeling each aspect of the features of chemical reactions leads to a complex system that must be designed upfront for future expansion as more or less detail is added or removed.

2 Phase 2: Multicomponent Modeling system

2.1 Features of Batteries

AI and machine learning will be applied to learn the distributed properties of chemistry models at various levels. Here features and properties are used to describe the various aspects of materials, reactions of those materials, batteries, and metrics of performance. Hidden features which are not discovered or named are accounted for in the AI model as hidden nodes which cannot be sampled or observed. The following are features of materials are available from the materials science project database. A simple common chemical compound such as H_2O can have over 20 different distinct entries representing the different phases and shapes of the material.

Elements	Density	Stoichiometry	Ionization energy
Bond types	Symmetry group	Magnetic moment	Formation energy
Oxidation states	Band Gap	Lattice parameters	Bond lengths

The following features are selected from the sets of materials and physical constraints. Even if every feature variable domain is highly restricted the combinations grow exponentially in this example:

$$O(4^N * 4^R)$$

Anode material	Cathode material	Charge carrier	Charge holder
Shape	Volume	Surface	Interface

The set of reaction features is the greatest unknown as some of the values must be derived from analysis of experimental data, such as activation energy with respect to catalysts over time. These features can currently be learned from book material and tested against from inferred data. They cannot be directly sampled in the laboratory so they will be modeled as internal variables that can be examined.

Half-cell potential	Reduction potential	Oxidation potential	Activation Energy
Catalyst	Inhibitor	Enthalpy	

The next set of features is also commonly profiled with respect to batteries specifically. These features can only be sampled from a complete complex systems. These features can be shown to influence the other features, such as raising the temperature changes the internal resistance which changes the discharge and charge rates. The features also vary with respect to time and charge cycles.

Discharge Rate	Charge Rate	Discharge efficiency	Charge efficiency
Temperature	Voltage	Resistance	Amperage
Time to charge	Time to discharge	Enthalpy	Entropy
Power density	Shelf life	Charge cycles	Operating Temp

3 Phase 3: Data Gathering

After proving that the models and simulation produce results similar to text book examples of the given features the data gathering phase of the project is ready to proceed. Sample batteries each with different specific chemical reactions will be purchased and analyzed. The specific goal would be to have a total spanning set of battery reactions that cover the commercially viable elements, approximately 39 different batteries with different elements. 28 which are available today. The characteristics and parameters will be used as training data for the modeling simulation AI during learning mode. Several batteries will need to be saved to validate that predicted results match real experimental results within acceptable margins of error. The simulation model will contain multitudes of abstraction layers which each have approximate eigenvalue weights that are able to encode the hidden parameters of battery construction.

Common name	anode	cathode	electrolyte
Zinc-Carbon	Zn	MnO_2	NH_4Cl, $ZnCl_2$
Magnesium	Mg	MnO_2	$MgBr_2$, $Mg(ClO_4)$
Manganese Dioxide	Zn	MnO_2	KOH
Mercuric Oxide	Zn	HgO	KOH, $NaOH$
Cadmium Mercury	Cd	HgO	KOH
Silver Oxide	Zn	Ag_2O, AgO	KOH , $NaOH$
Zinc Air	Zn	O_2	KOH
Lithium	Li	SO_2	Organic solvent salt solution
Lithium	Li	SOC	$SOCl_2$, $AlCl_4$
Lithium	Li	MnO_2	Organic solvent salt solution
Lithium	Li	FeS_2	Organic solvent salt solution
Lithium	Li	I_2	Solid
Lead Acid	Pb	PbO_2	H_2SO_4
Nicad	Cd	$NiOOH$	KOH
Ni-Iron	Fe	$NiOOH$	KOH
Silver-Zinc	Zn	AgO	KOH
Silver-Cadmium	Cd	AgO	KOH
Nickel Hydride	H_2	$NiOOH$	KOH
Metal-Hydride	M_xH	$NiOOH$	KOH
Manganese Recharge	Zn	MnO_2	KOH
Lithium	C	$LiCoO2$	organic solvent