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Predicting Li-ion Battery Performance for Impurity-doped NMC Cathodes Using Deep Learning

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Abstract. With the electric vehicle (EV) market expansion and the energy sector's shift towards electrification, the demand for battery metals, including lithium (Li), cobalt (Co), and nickel (Ni), is set to surpass supply. A critical knowledge gap exists in the purity standards for battery precursors and the impact of impurities on battery performance. Addressing this, our study employs a Deep Machine Learning (DL) based multi-objective optimization approach to interpret the relationship between metal impurities in domestic battery resources and their effects on battery performance. We analyze experimental data from Li-ion batteries with NMC (Nickel-Manganese-Cobalt oxide) cathodes over 1000 cycles, representing approximately ~6-8 months of operation, to establish a baseline of performance without impurities. Leveraging this data, we develop a Physics-Informed Deep Learning (PIDL) framework to extend our findings to cases that include metal impurities (*e.g.,* Fe, Cu, Al) ranging from (0.001 - 0.01) %, respectively. By incorporating physics-based features, our PIDL model can accurately estimate the performance of NMC cathodes doped with various metal impurities to provide rapid design decisions. This research paves the way for informed decisions in Li-ion battery material design and optimization, ensuring the sustainable growth of the EV market and the broader energy sector.

Keywords: Li-ion battery, NMC(nickel-manganese-cobalt oxide) cathodes, metal impurities, machine learning, electric vehicle(EV)

Physical Model, Methodology and Governing Equations

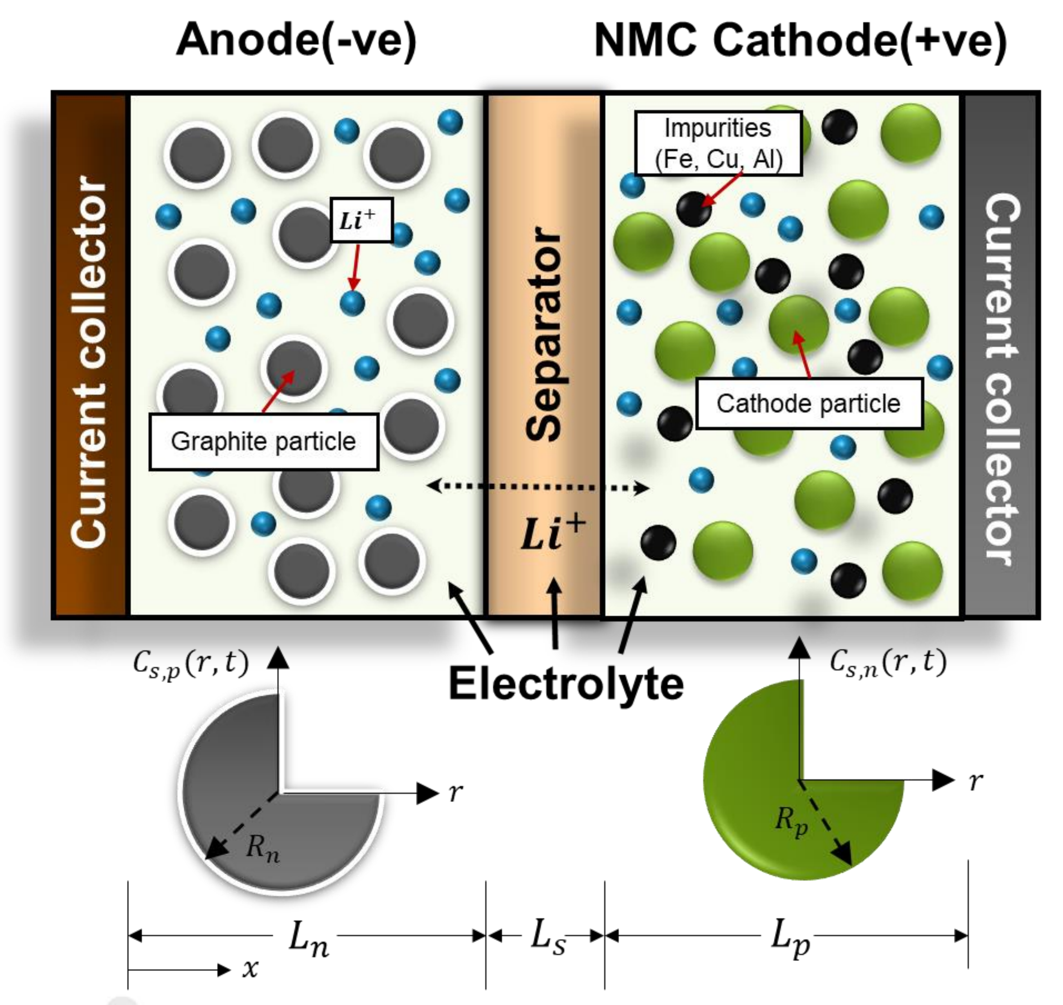
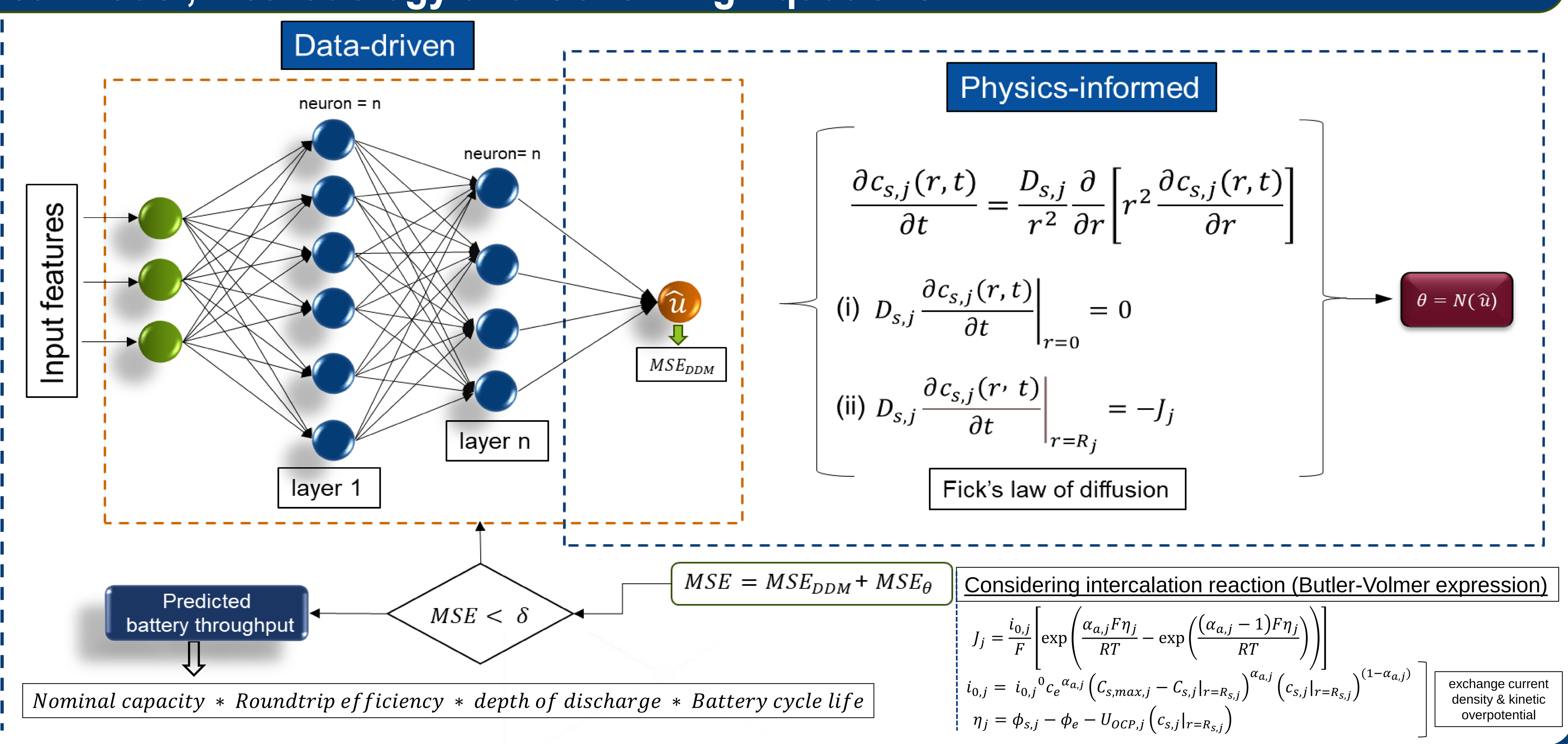


Fig 1. Schematic of a Li-ion battery with impurity doped NMC cathode where Impurity metals are – Fe, Cu and Al



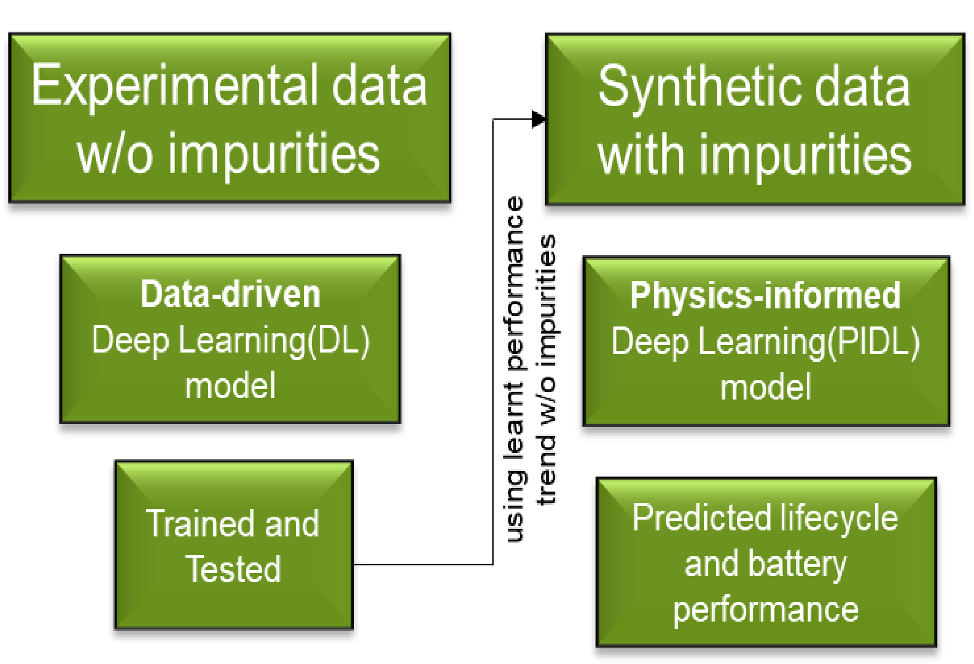
Data Generation

- ❑ Cathode type: NMC622 (0.6 Ni : 0.2 Mn : 0.2 CoO_2)
- ❑ Experimental Data without Impurities:
  - Run time for 1 battery for lifetime of 750-1100 cycles is around 6-8 months
  - Datasets (training features) mentioned in Table 1 have been captured and obtained from **battery-pro** software
  - Battery throughput i.e., battery performance is calculated using eqn. (1), below

$$Battery\ throughput = Nominal\ capacity * Roundtrip\ efficiency * depth\ of\ discharge * Battery\ cycle\ life \quad (1)$$

- ❑ Synthetic datasets with impurities
  - Impurity metals: Iron(Fe), Copper(Cu), Aluminum(Al)
  - Impurity percentages for each metal – 0.001%, 0.005%, 0.01%
  - Based on the information obtained for battery performance w/o impurities, synthetic datasets have been generated to train a PIDL model solving the governing equations and boundary conditions.
  - To solve the physics–based equations, we obtain the required **"features"** stated in Table 2. based on literature datasets.

Training and Testing



Results and Discussions

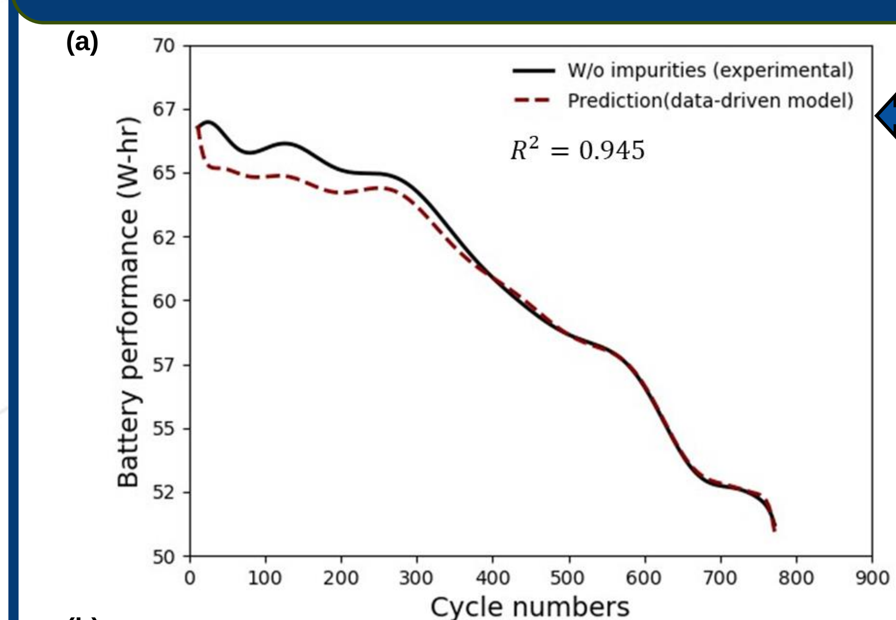


Fig 2. Battery performance for NMC cathode **without impurities**

Variation of battery performance over battery lifetime, plotted for experimental datasets without impurities in NMC cathodes. A data-driven Deep Learning(DL) model has been trained for the experimental data and its predictability has been tested using R-squared metric.

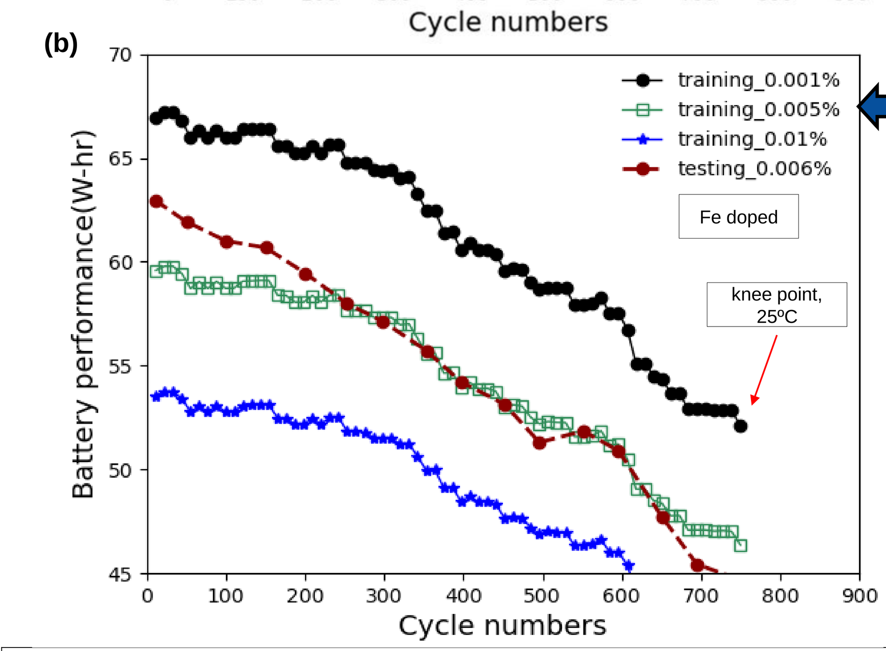


Fig 3. Battery performance for NMC cathode with **Fe(iron) impurities**

Variation of battery performance over battery lifetime. A Physics-informed Deep Learning (PIDL) model has been trained for three(3) different sets of Fe-impurity datasets and tested for 0.006% Fe-impurity-doped NMC cathode dataset for battery lifetime prediction.

Feature Names and Feature numbers

1	Cycle C	16	ESR	31	dc_sj_dt
2	Rec	17	VAR6	32	dc_sj_dr
3	Cycle P	18	VAR10	33	D_s
4	Step	19	impurity percentage	34	F_constant
5	Capacity (A-hr)	20	atomic radius	35	R_p
6	Energy (W-hr)	21	electronegativity	36	R_n
7	Current (A)	22	density	37	porosity_p
8	Voltage (V)	23	crystal structure(lattice constant)	38	porosity_n
9	ES	24	Thermal expansion co-efficient	39	Volume Fraction(+ve)
10	I Range	25	electrode potential	40	Volume Fraction(-ve)
11	S.Capacity (Ah/g)	26	volumetric capacity of impurities (Ah/cm^3)	41	Electrode Volume
12	Power (W)	27	Capacity change based on Cathode dimension	42	Symmetry factor
13	Loop	28	C_s	43	Exchange Current Density
14	Resistance	29	radial coordinate	44	Kinetic overpotential(mV)
15	Conductivity	30	time		

Table 1. Input and physics-based features for training both DL and PIDL model.

- Input features have been obtained from experimental data and used in DL model.
- Physics-based features (no.19-44) have been added to enhance training in PIDL model.

Conclusion

- **Accelerated prediction** - Our developed PIDL framework can precisely predict the overall lifecycle of a Li-ion battery with impurity doped NMC cathodes in seconds.
- **Design decision** - It can help us to achieve quick and informed design decision to optimize battery performance.
- **Cost and Time** – PIDL models can significantly reduce costs by reducing experimental timeline for a single battery from ~6-8 months to a few seconds and by minimizing expenses involved in refining metallic materials.

Obstacles and Future Direction

- **Insufficient training datasets** – Due to prolonged duration of our experiments, we lacked sufficient training data to effectively train our deep learning model. Hence, we created **synthetic placeholder datasets** to evaluate the effect of impurities for PIDL model development, training and testing.
- **Future direction –**
  - Use **electrochemical impedance spectroscopy** data for solving the governing equations for the PIDL model.
  - Validate and optimize our model with each new acquisition of experimental data.
  - Extend the performance prediction for other metal impurities (e.g., Cu, Al, Mg or combination of metal impurities)
  - Use the model for inverse design and multi-objective optimization (e.g., cost analysis)

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