Multiscale modelling of novel solid oxide electrolysis cell materials using machine learned based Approach

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- Molecular dynamics (MD) simulation for oxide ion transport in YSZ and Brownmillerites for SOECs.
- Coupling of MD to electrochemical modeling and transport modelling for cell level efficiency.

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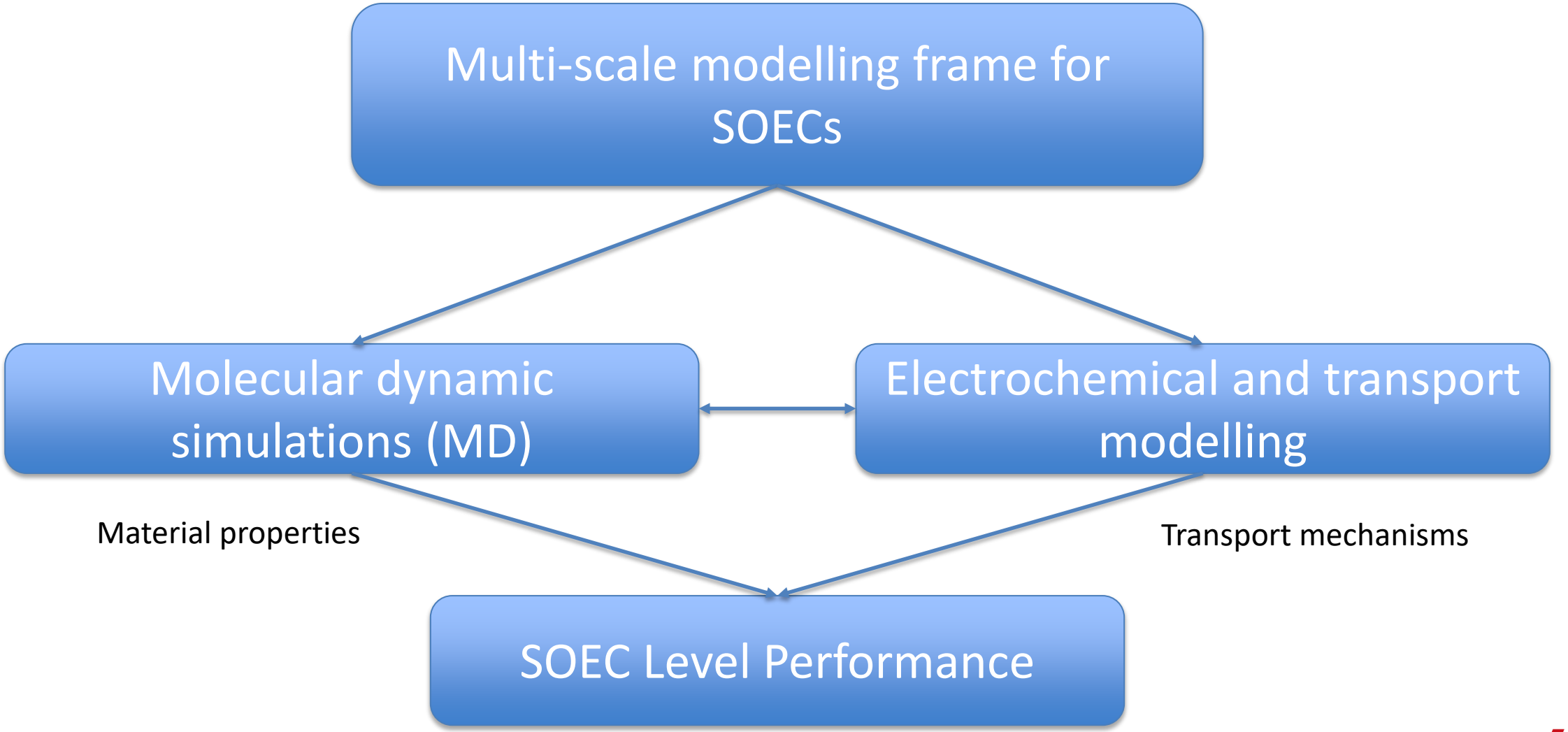
Multi-scale modelling frame for SOECs
Molecular dynamic simulations (MD)
Electrochemical and transport modelling
Material properties
Transport mechanisms
SOEC Level Performance

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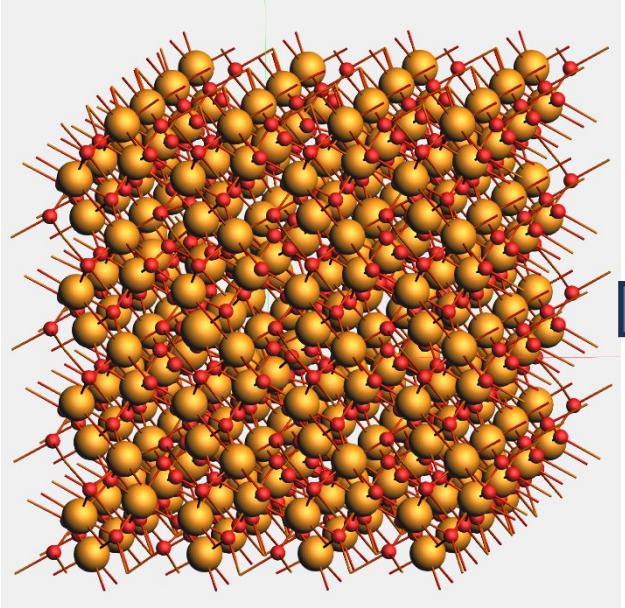
Modelling of YSZ



3x3x3 Supercell of YSZ 8%

ML Interatomic potentials

$$D = \frac{1}{2d}\lim_{t\to\infty}\frac{d}{dt}\left\langle |r(t) - r(0)|^2 \right\rangle$$

$$\sigma = \frac{nq^2D}{k_BT}$$

$$D(T) = D_0 \exp\left(-\frac{E_a}{k_BT}\right)$$

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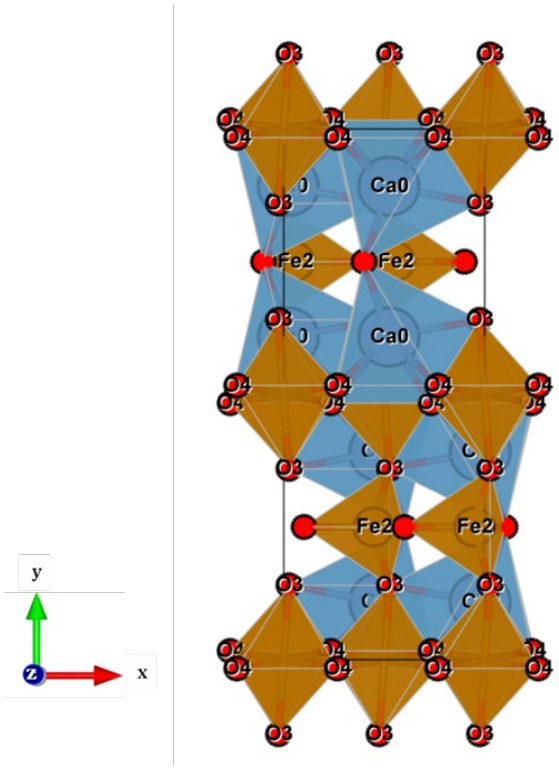
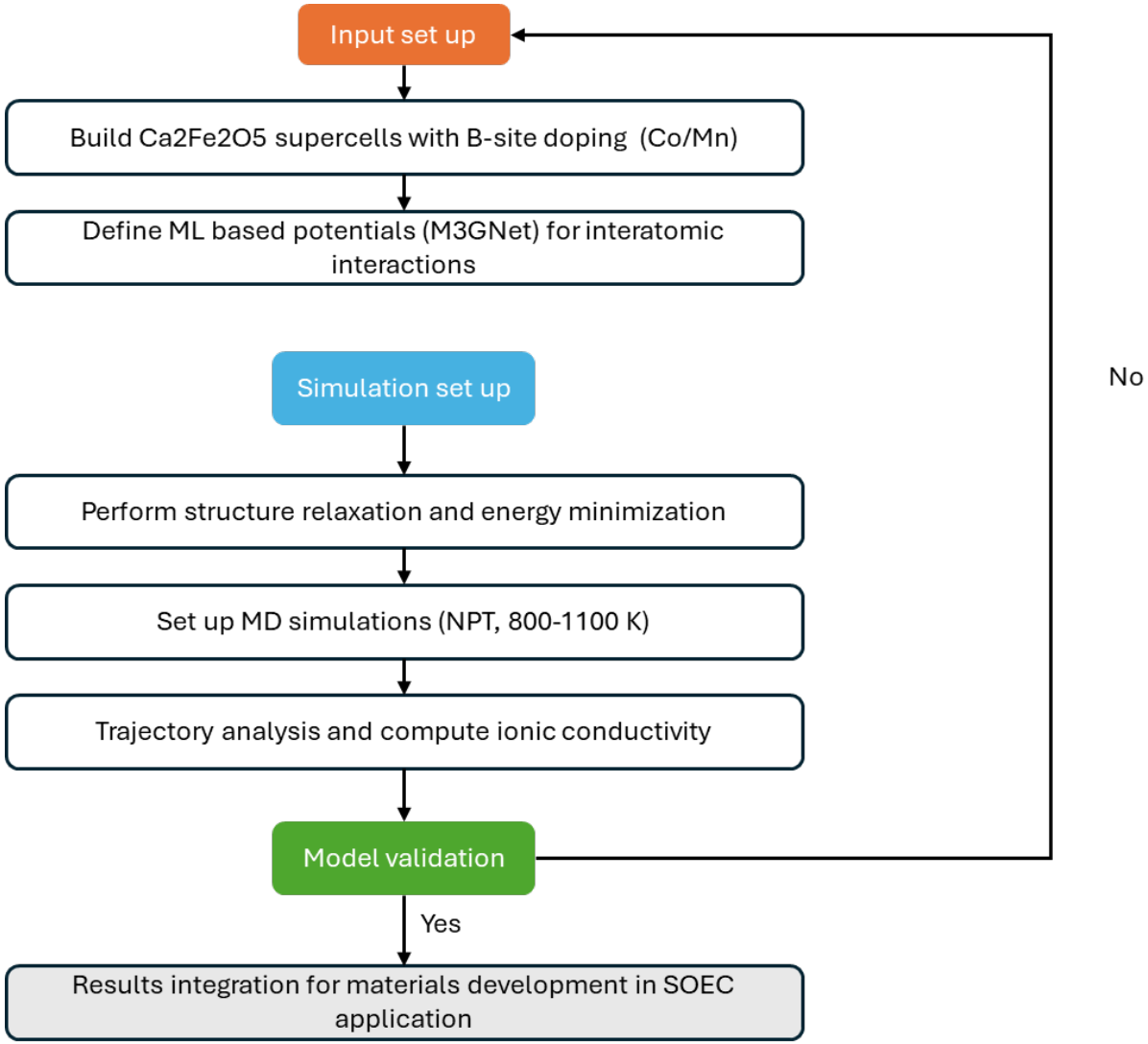
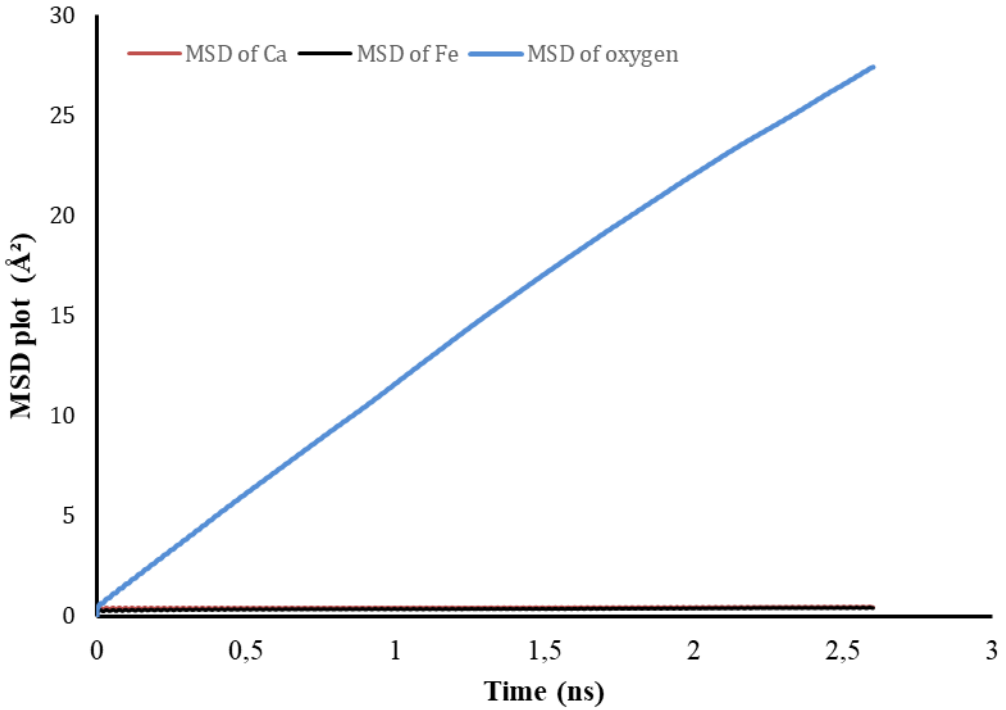
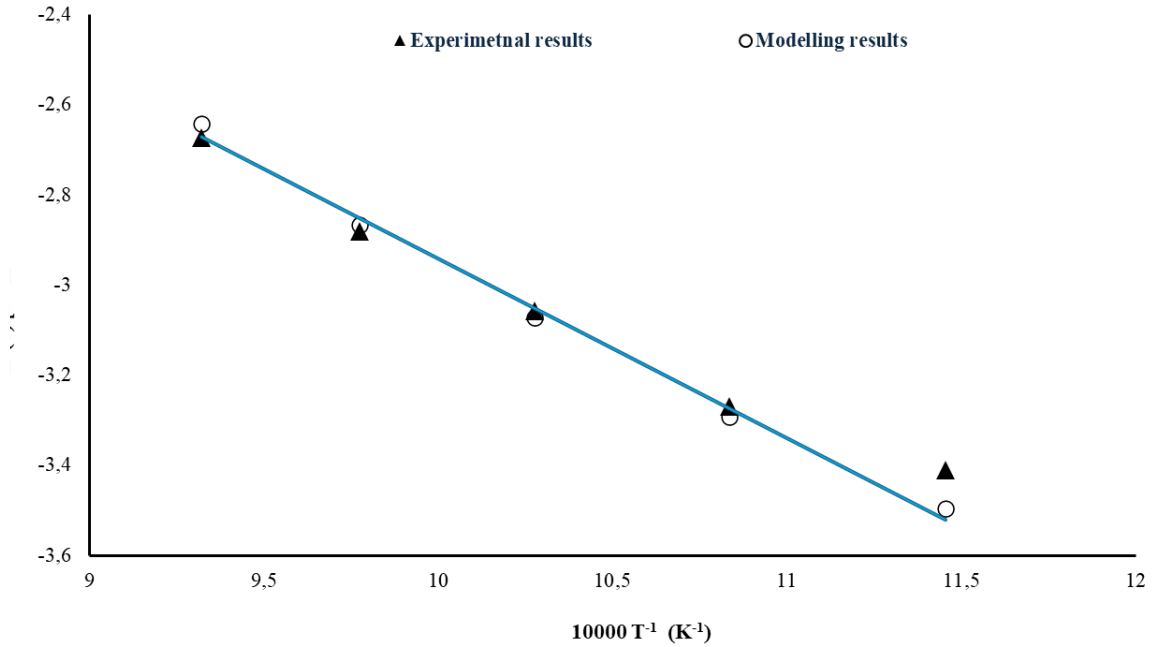

y
x
Ca0
Fe2
O3
O4


Input set up
Build Ca2Fe2O5 supercells with B-site doping (Co/Mn)
Define ML based potentials (M3GNet) for interatomic interactions
Simulation set up
Perform structure relaxation and energy minimization
Set up MD simulations (NPT, 800-1100 K)
Trajectory analysis and compute ionic conductivity
Model validation
No
Yes
Results integration for materials development in SOEC application

Model validation for the ionic conductivities of Brownmillerites





https://doi.org/10.1016/j.ijhydene.2019.01.164

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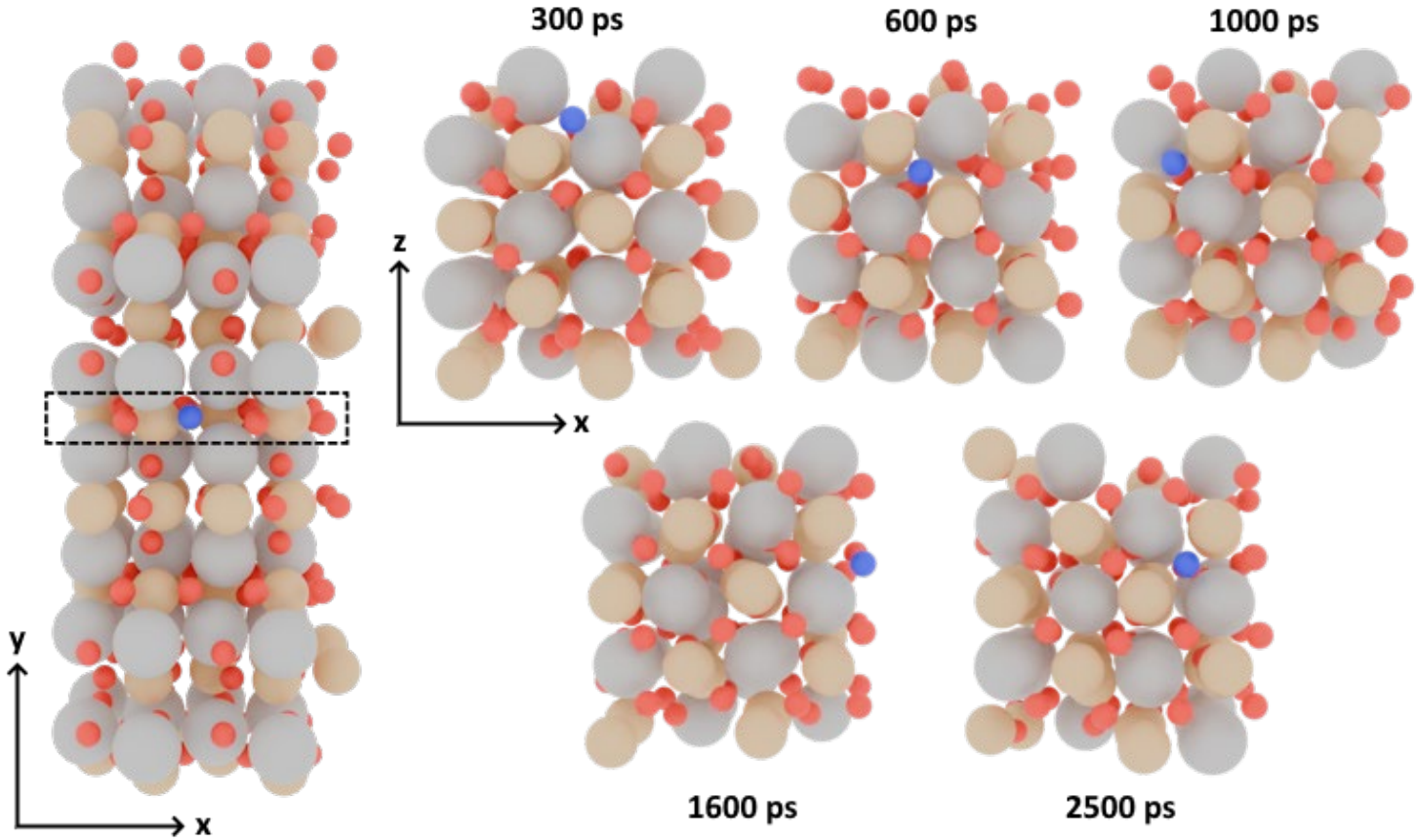
NOVEL ELECTRODE COATINGS AND INTERCONNECT FOR SUSTAINABLE AND REUSABLE SOEC



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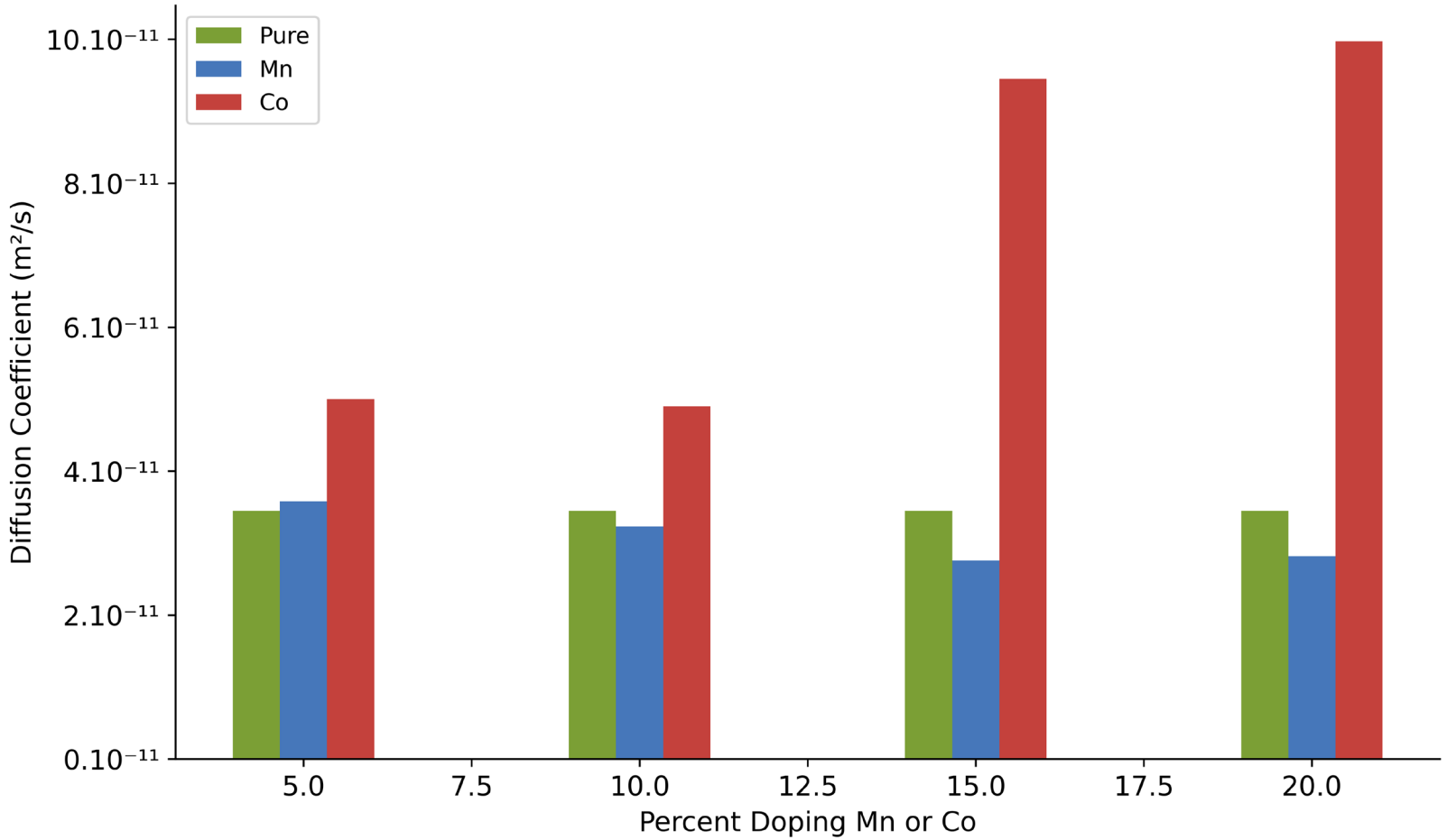

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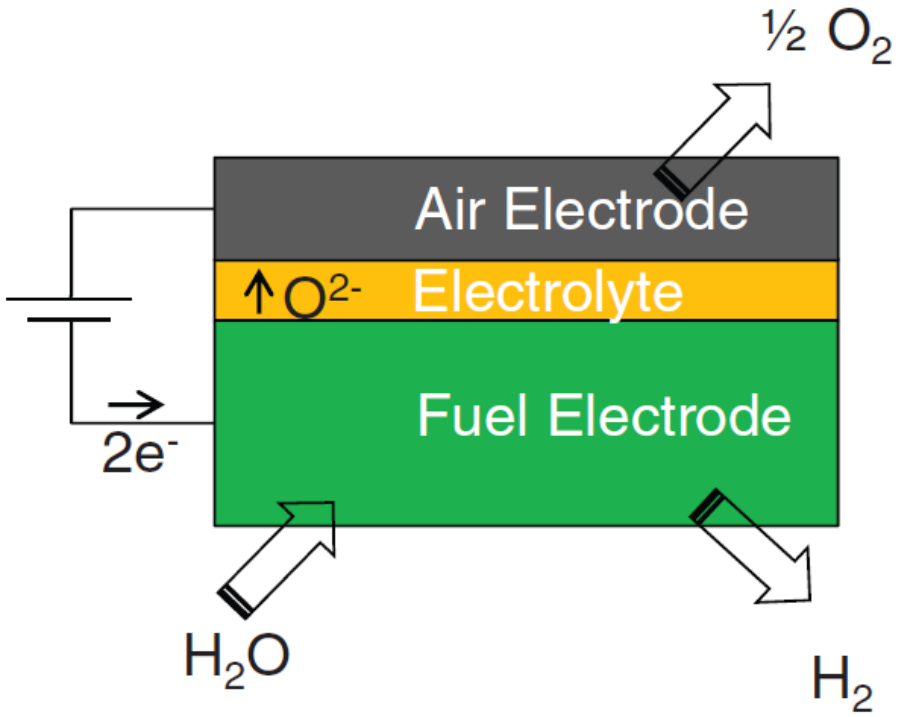
Electrochemical model (0 D) for SOEC/SOFCs

- The model based on Physical laws:
  - Butler-volmer Equation
  - Ficks Law
  - Ohm's Law



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$$U_{\text{Cell}} = U_{\text{OCV}} - \left(\eta_{\text{ohm}} + \eta_{\text{act,an}} + \eta_{\text{act,cat}} + \eta_{\text{conc,an}} + \eta_{\text{conc,cat}}\right)$$

$$U_{\text{OCV}}(T) = U_0(T) - \frac{RT}{2F}\ln\left(\frac{p\text{H}_2\text{O}_{\text{an}}}{p\text{H}_2,\text{an} \cdot \sqrt{p\text{O}_2,\text{cat}}}\right)$$

$$\eta_{\text{ohm}} = j \cdot \sum_k R_k = j \cdot R_{\text{ohm}}$$

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$$\eta_{\text{ohm}} = j \cdot \sum_k R_k = j \cdot R_{\text{ohm}}$$

$$R_{\text{ohm}} = \sum_k \frac{L_k}{\left(\frac{1}{\sigma_{\text{ion},k}} + \frac{1}{\sigma_{\text{el},k}}\right)}$$

$$R_{\text{cat}} = \frac{L_{\text{cat}}}{\left(\frac{1}{\sigma_{\text{ion,cat}}} + \frac{1}{\sigma_{\text{el,cat}}}\right)}$$

$$R_{\text{an}} = \frac{L_{\text{an}}}{\left(\frac{1}{\sigma_{\text{ion,an}}} + \frac{1}{\sigma_{\text{el,an}}}\right)}$$

$$R_{\text{elyte}} = \frac{L_{\text{elyte}}}{\sigma_{\text{ion,elyte}}}$$

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$$p\mathrm{H}_2^{TPB,\mathrm{an}} = p\mathrm{H}_{2,\mathrm{an}} - \frac{RTL_{\mathrm{an}}}{2FD_{\mathrm{H2}}^{\mathrm{eff}}P_0} \cdot j$$

$$p\mathrm{H}_2\mathrm{O}^{TPB,\mathrm{an}} = p\mathrm{H}_2\mathrm{O}_{\mathrm{an}} + \frac{RTL_{\mathrm{an}}}{2FD_{\mathrm{H2O}}^{\mathrm{eff}}P_0} \cdot j$$

$$p\mathrm{O}_2^{TPB,\mathrm{cat}} = p\mathrm{O}_{2,\mathrm{cat}} - \left(\frac{p_{\mathrm{tot}} - p\mathrm{O}_{2,\mathrm{cat}}}{p_{\mathrm{tot}}}\right) \cdot \frac{RTL_{\mathrm{cat}}}{4FD_{\mathrm{O2}}^{\mathrm{eff}}P_0} \cdot j$$

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$$\eta_{\text{conc,an}} = \frac{RT}{2F}\ln\left(\frac{p\mathrm{H_2O}_{\text{an}}^{TPB}\cdot p\mathrm{H_{2,an}}}{p\mathrm{H_2O_{an}}\cdot p\mathrm{H_2}^{TPB,\text{an}}}\right)$$

$$\eta_{\text{conc,an}} = \frac{RT}{2F}\ln\left(\frac{1+\frac{RTL_{\text{an}}}{2FD_{\mathrm{H_2O}}^{\text{eff}}p\mathrm{H_2O_{an}}P_0}\cdot j}{1-\frac{RTL_{\text{an}}}{2FD_{\mathrm{H_2}}^{\text{eff}}p\mathrm{H_{2,an}}P_0}\cdot j}\right)$$

$$\eta_{\text{conc,cat}} = \frac{RT}{4F}\ln\left(\frac{p\mathrm{O_{2,cat}}}{p\mathrm{O_2}^{TPB,\text{cat}}}\right)$$

$$\eta_{\text{conc,cat}} = \frac{RT}{4F}\ln\left(\frac{1}{1-\frac{RTL_{\text{cat}}(1-p\mathrm{O_{2,cat}}/p_{\text{tot}})}{4FD_{\mathrm{O_2}}^{\text{eff}}p\mathrm{O_{2,cat}}P_0}\cdot j}\right)$$

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$$j = j_{0,\mathrm{el}} \left[\exp\left(\frac{\alpha_{\mathrm{el}}\, n_e F \eta_{\mathrm{act,el}}}{RT} \right) - \exp\left(\frac{-(1-\alpha_{\mathrm{el}})\, n_e F \eta_{\mathrm{act,el}}}{RT} \right) \right]$$

$$j_{0,\mathrm{an}} = \gamma_{\mathrm{an}} \left(p\mathrm{H}_2^{TPB,\mathrm{an}} \right)^a \left(p\mathrm{H}_2\mathrm{O}^{TPB,\mathrm{an}} \right)^b \exp\left(\frac{-E_{\mathrm{act,an}}}{RT} \right)$$

$$j_{0,\mathrm{cat}} = \gamma_{\mathrm{cat}} \left(p\mathrm{O}_2^{TPB,\mathrm{cat}} \right)^m \exp\left(\frac{-E_{\mathrm{act,cat}}}{RT} \right)$$

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Electrolyte YSZ	Activation energy (KJ/mol)	Pre-exponential factor (S.K/m)	Arrhenius fit
MD based	54	$1.93x10^5$	$\sigma_{MD}(T) = \frac{1.93x105}{T}.\exp(-\frac{54000}{RT})$
Empirical expression (exp data) Resistance	$0.265 + 0.24 \times 10^6.\exp(-0.0125T)\ (\frac{ohm}{cm^2})$		

https://doi.org/10.1016/j.enconman.2023.117778

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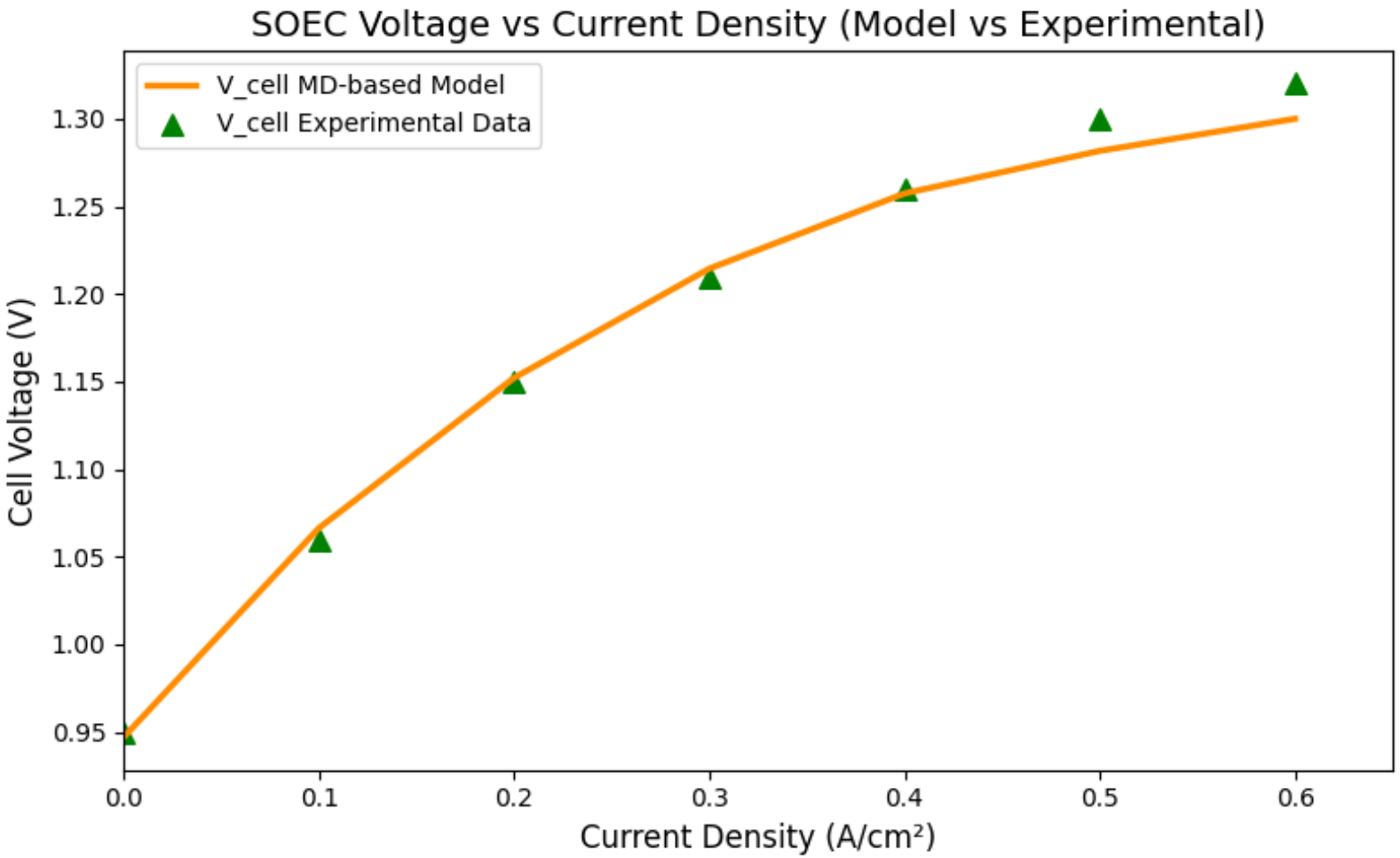

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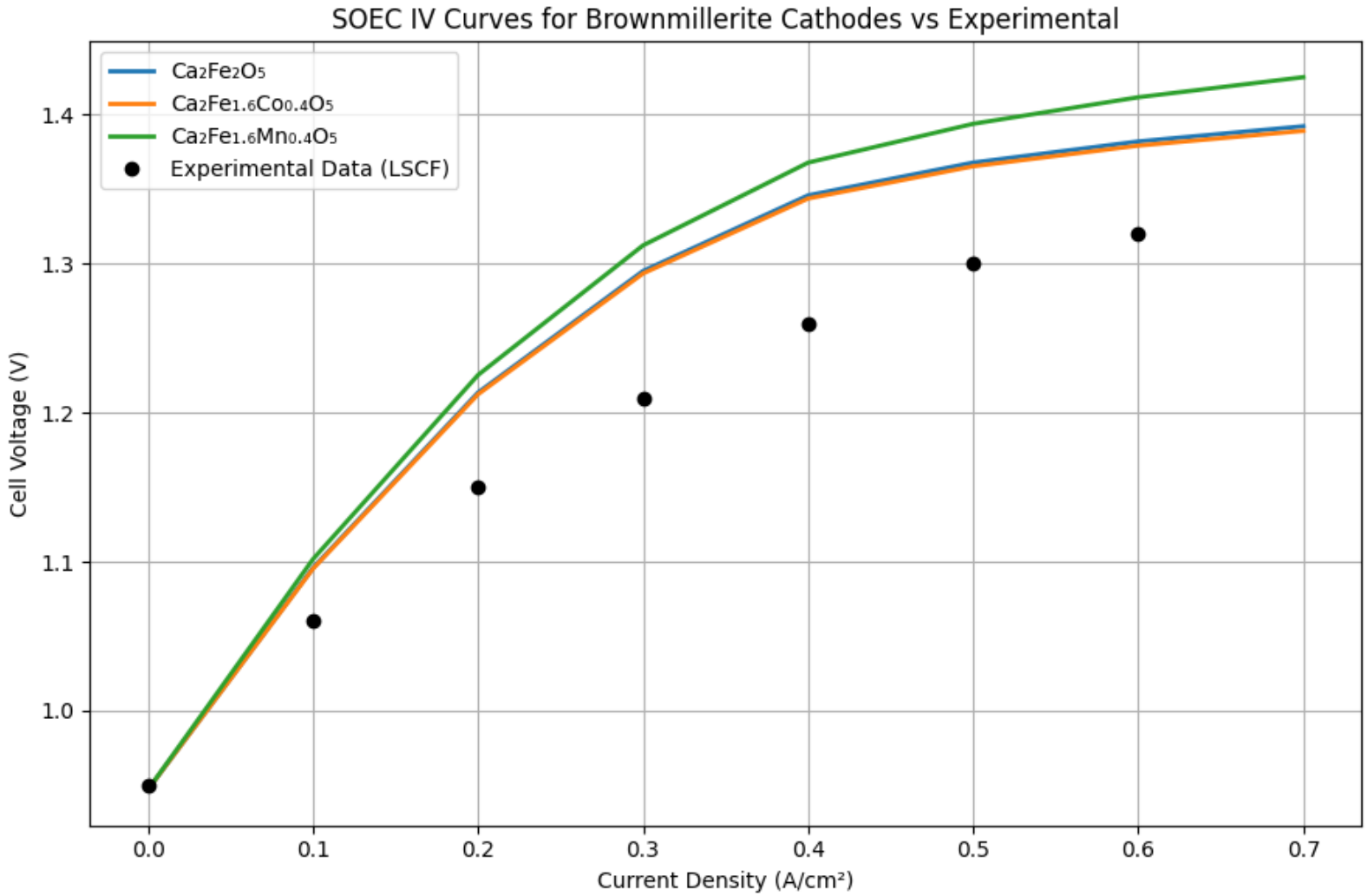
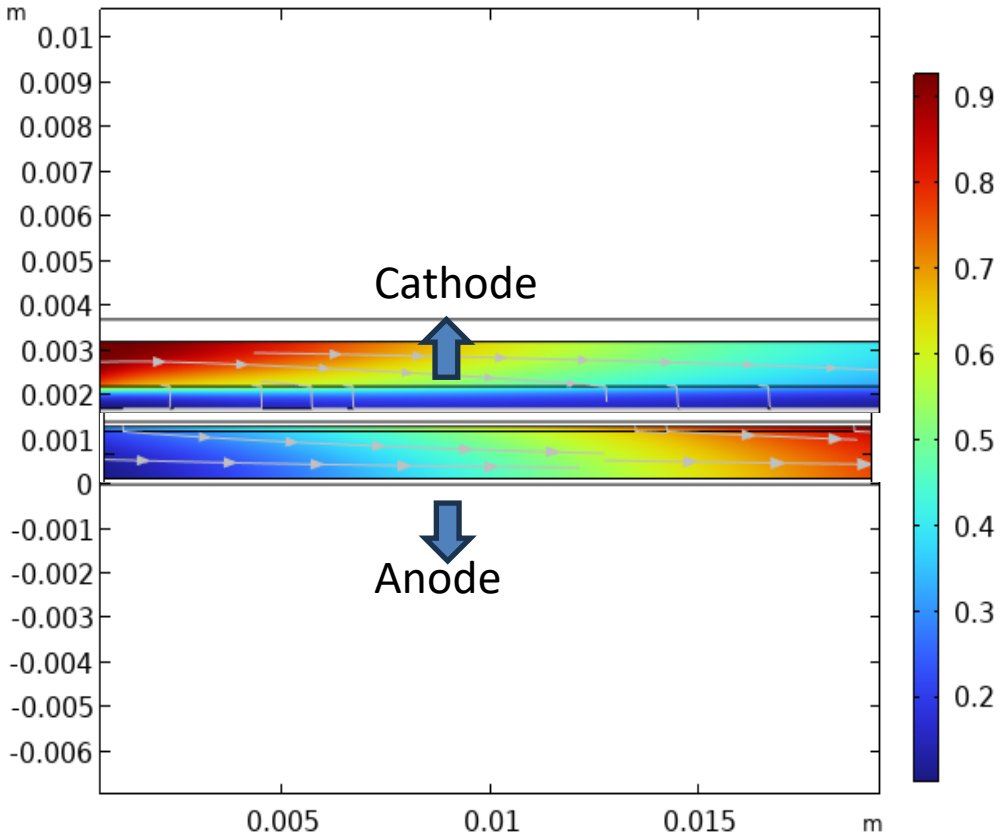
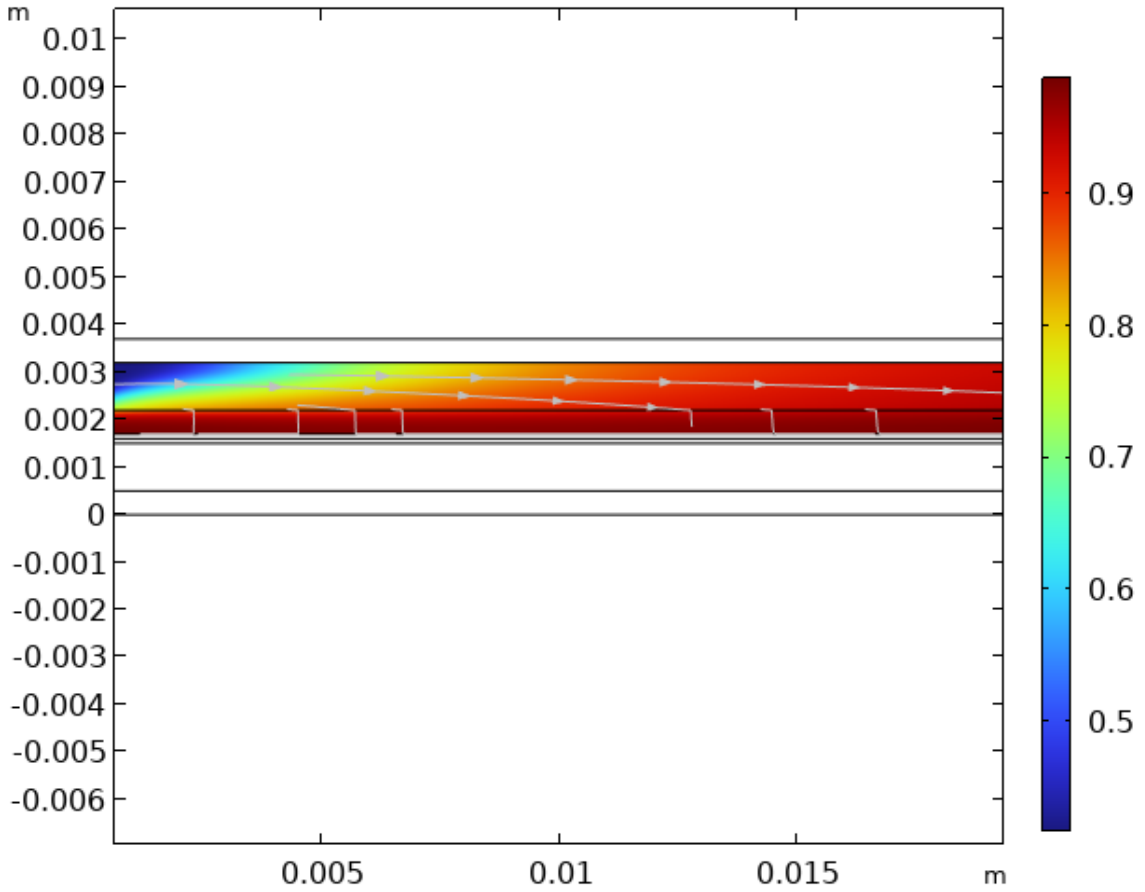

SOEC IV Curves for Brownmillerite Cathodes vs Experimental
Ca2Fe2O5
Ca2Fe1.6Co0.4O5
Ca2Fe1.6Mn0.4O5
Experimental Data (LSCF)
Cell Voltage (V)
1.0
1.1
1.2
1.3
1.4
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
Current Density (A/cm²)

2D transport modelling



(a) Steam consumption and oxygen production



(a) Hydrogen production

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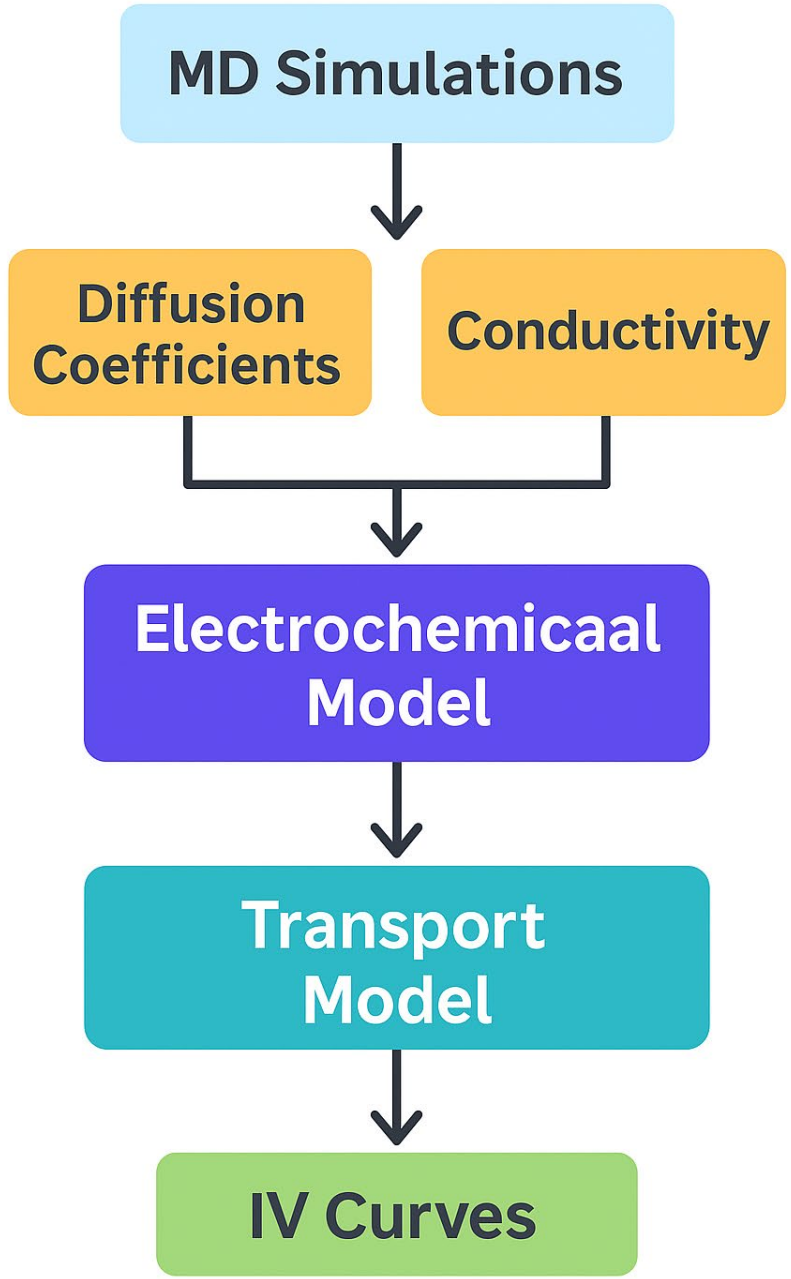
MD Simulations
Diffusion Coefficients
Conductivity
Electrochemicaal Model
Transport Model
IV Curves

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