**Calculation code of interfacial resistance based on ligand-field and space-charge layer**

**V 1.0**

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**Contents**

[**1.** **How to reproduce the results in the manuscript?** 3](#_Toc137588234)

[**1.1 Code** 3](#_Toc137588235)

[**1.2 Data** 3](#_Toc137588236)

[**1.3 Result** 3](#_Toc137588237)

[**2.** **Code manual for interfacial resistance calculations based on ligand-field and space-charge layer** 17](#_Toc137588238)

[**2.1 Introduction** 17](#_Toc137588239)

[**2.2 Hardware and software requirements** 23](#_Toc137588240)

[**2.3 Input file** 24](#_Toc137588241)

[**2.4 Running the code** 25](#_Toc137588242)

[**2.5 Output File** 25](#_Toc137588243)

[**2.6 Example** 26](#_Toc137588244)

[**3.** **Reference** 27](#_Toc137588245)

1. **How to reproduce the results in the manuscript?**

**1.1 Code**

There are four files for the code. “\_\_init\_\_.py” is the main module for the calculation of interfacial resistance. “constants.py” collect the corresponding physical constants, such as Boltzmann constant (1.381×10‒23 J K−1), molar gas constant (8.314 J mol−1 K−1), elementary charge (1.602×10‒19 C), vacuum permittivity, and Avogadro constant (6.022×1023 mol‒1). “input\_parameter.py” is used to assign the type of cathode or coating, and the parameters of the solid electrolyte (SE), *e.g.*, surface area (*A*), permittivity (), diffusivity (*D*), and bulk electric-potential (). “input\_mcfss.py” is used to assign the required electric-potential parameters. Here the interfacial electric-potential difference is described by the proposed MCFSS (the detailed description and obtaining method are shown in **2.1** and **2.3,** respectively) or electric band values.

**1.2 Data**

The “input\_parameter.py” and “input\_mcfss.py” files contain the initial input parameters in the manuscript.

The “input\_mcfss.py” file contains the electric-potential parameters of 31 cathode and coating materials, involving LiMnO2, LiFeO2, LiCoO2, LiNiO2, NCM333, NCM523, NCM622, NCM811, Li2MnO3, Li1+*x*V3O8, LiMn2O4, LiN0.5Mn1.5O4, LiFePO4, Li4Ti5O12, Li2ZrO3, LiNbO3, LiTaO3, LiTiS2, LiVS2, LiCrS2, LiMnS2, LiFeS2, LiCoS2, LiNiS2, LiCuS2, LiZrS2, LiNbS2, LiMoS2, LiHfS2, LiTaS2, LiWS2 and Li2V0.5Cr1.5S4.

The “input\_parameter.py” file contains the parameters of 10 SE materials (mentioned in **1.1**), concluding Li10GeP2S12, Li3PS4, Li6PS5Cl, Li7La3Zr2O12, Li0.33La0.56TiO3, Li3OCl, LiTi2(PO4)3, Li2PO2N, Li3YCl6 and Li3InCl6.

**1.3 Result**

Our code is based on python. When run the “\_\_init\_\_.py” module, the code will automatically read the relevant parameters of the cathodes, coatings, and SEs in the “input\_parameter.py” and “input\_mcfss.py” files. In the end, the output file “scl\_resistance.csv”, containing the interfacial resistance and the SE, will be generated in the current folder. The results in the manuscript are shown in Table 1.

**Table 1**. The Miller index, band energy-level difference (), resistance calculated based on (), normalized resistance calculated based on (), SCL resistance (), normalized SCL resistance (), and experimental interfacial resistance for 310 cathode (or coating)/SE interfaces.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Type | Cathode or coating | SE | (Ω) |  | (Ω) |  |
| Oxide  cathode | LiMnO2 | Li10GeP2S12 | 2.664×1013 | 4.879×10−9 | 5.393×1011 | 2.978 |
| LiFeO2 | 4.058×1018 | 7.432×10−4 | 7.560×1011 | 4.175 |
| LiCoO2 | 5.460×1021 | 1.000 | 1.811×1011 | 1.000 |
| LiNiO2 | 1.222×1017 | 2.238×10−5 | 2.169×1011 | 1.198 |
| NCM333 | 2.017×108 | 3.694×10−14 | 5.414×1012 | 29.901 |
| NCM523 | 1.776×1010 | 3.252×10−12 | 1.134×1013 | 62.641 |
| NCM622 | 4.618×1010 | 8.457×10−12 | 3.269×1013 | 1.805×102 |
| NCM811 | 4.574×1010 | 8.377×10−12 | 6.762×1013 | 3.734×102 |
| Li2MnO3 | 7.406×1021 | 1.356 | 5.384×1010 | 0.297 |
| Li1+*x*V3O8 | 1.528×1022 | 2.798 | 1.871×1011 | 1.033 |
| LiMn2O4 | 3.137×1016 | 5.746×10−6 | 8.629×1010 | 0.477 |
| LiNi0.5Mn1.5O4 | 1.404×1024 | 2.571×102 | 6.882×1012 | 38.012 |
| LiFePO4 | 4.411×108 | 8.079×10−14 | 5.229×108 | 2.887×10−3 |
| Oxide  coating | Li4Ti5O12 | 3.559×108 | 1.962×10−16 | 5.114×108 | 2.824×10−3 |
| Li2ZrO3 | 1.465×109 | 8.076×10−16 | 5.639×108 | 3.114×10−3 |
| LiNbO3 | 3.982×108 | 2.195×10−16 | 5.130×108 | 2.833×10−3 |
| LiTaO3 | 4.137×108 | 2.281×10−16 | 6.213×108 | 3.431×10−3 |
| Sulfide  cathode | Li*x*TiS2 | / | / | 1.915×108 | 1.057×10−3 |
| Li*x*VS2 | 1.853×108 | 1.023×10−3 |
| Li*x*CrS2 | 1.702×108 | 9.397×10−4 |
| Li*x*MnS2 | 1.812×108 | 1.000×10−3 |
| Li*x*FeS2 | 2.188×108 | 1.208×10−3 |
| Li*x*CoS2 | 2.005×108 | 1.107×10−3 |
| Li*x*NiS2 | 1.899×108 | 1.049×10−3 |
| Li*x*CuS2 | 1.381×108 | 7.629×10−4 |
| Li*x*ZrS2 | 2.442×108 | 1.348×10−3 |
| Li*x*NbS2 | 1.955×108 | 1.080×10−3 |
| Li*x*MoS2 | 1.647×108 | 9.097×10−4 |
| Li*x*HfS2 | 1.958×108 | 1.081×10−3 |
| Li*x*TaS2 | 1.905×108 | 1.052×10−3 |
| Li*x*WS2 | 1.476×108 | 8.149×10−4 |
| Li2*x*V0.5Cr1.5S4 | 2.654×108 | 1.466×10−3 |
| Oxide  cathode | LiMnO2 | Li3PS4 | 8.813×1014 | 1.614×10−7 | 1.784×1013 | 98.531 |
| LiFeO2 | 1.343×1020 | 2.459×10−2 | 2.501×1013 | 1.381×102 |
| LiCoO2 | 1.806×1023 | 33.081 | 5.990×1012 | 33.081 |
| LiNiO2 | 4.043×1018 | 7.405×10−4 | 7.174×1012 | 39.621 |
| NCM333 | 6.673×109 | 1.222×10−12 | 1.791×1014 | 9.891×102 |
| NCM523 | 5.874×1011 | 1.076×10−10 | 3.752×1014 | 2.072×103 |
| NCM622 | 1.528×1012 | 2.798×10−10 | 1.081×1015 | 5.972×103 |
| NCM811 | 1.513×1012 | 2.771×10−10 | 2.237×1015 | 1.235×104 |
| Li2MnO3 | 2.450×1023 | 44.871 | 1.781×1012 | 9.836 |
| Li1+*x*V3O8 | 5.054×1023 | 92.562 | 6.188×1012 | 34.181 |
| LiMn2O4 | 1.038×1018 | 1.901×10−04 | 2.855×1012 | 15.773 |
| LiNi0.5Mn1.5O4 | 4.645×1025 | 8.507×103 | 2.277×1014 | 1.257×103 |
| LiFePO4 | 1.459×1010 | 2.673×10−12 | 1.730×1010 | 9.553×10−2 |
| Oxide  coating | Li4Ti5O12 | 1.177×1010 | 6.491×10−15 | 1.692×1010 | 9.344×10−2 |
| Li2ZrO3 | 4.847×1010 | 2.672×10−14 | 1.866×1010 | 0.103 |
| LiNbO3 | 1.317×1010 | 7.262×10−15 | 1.697×1010 | 9.373×10−2 |
| LiTaO3 | 1.369×1010 | 7.545×10−15 | 2.055×1010 | 0.114 |
| Sulfide  cathode | Li*x*TiS2 | / | / | 6.335×109 | 3.498×10−2 |
| Li*x*VS2 | 6.130×109 | 3.385×10−2 |
| Li*x*CrS2 | 5.630×109 | 3.109×10−2 |
| Li*x*MnS2 | 5.993×109 | 3.310×10−2 |
| Li*x*FeS2 | 7.238×109 | 3.997×10−2 |
| Li*x*CoS2 | 6.634×109 | 3.664×10−2 |
| Li*x*NiS2 | 6.283×109 | 3.470×10−2 |
| Li*x*CuS2 | 4.570×109 | 2.524×10−2 |
| Li*x*ZrS2 | 8.078×109 | 4.461×10−2 |
| Li*x*NbS2 | 6.469×109 | 3.572×10−2 |
| Li*x*MoS2 | 5.450×109 | 3.010×10−2 |
| Li*x*HfS2 | 6.476×109 | 3.576×10−2 |
| Li*x*TaS2 | 6.302×109 | 3.480×10−2 |
| Li*x*WS2 | 4.882×109 | 2.696×10−2 |
| Li2*x*V0.5Cr1.5S4 | 8.781×109 | 4.849×10−2 |
| Oxide  cathode | LiMnO2 | Li6PS5Cl | 4.433×1013 | 8.118×10−9 | 8.973×1011 | 4.956 |
| LiFeO2 | 6.752×1018 | 1.237×10−3 | 1.258×1012 | 6.947 |
| LiCoO2 | 9.085×1021 | 1.664 | 3.013×1011 | 1.664 |
| LiNiO2 | 2.033×1017 | 3.724×10−05 | 3.608×1011 | 1.993 |
| NCM333 | 3.356×108 | 6.147×10−14 | 9.008×1012 | 49.751 |
| NCM523 | 2.954×1010 | 5.411×10−12 | 1.887×1013 | 1.042×102 |
| NCM622 | 7.684×1010 | 1.407×10−11 | 5.439×1013 | 3.004×102 |
| NCM811 | 7.611×1010 | 1.394×10−11 | 1.125×1014 | 6.214×102 |
| Li2MnO3 | 1.232×1022 | 2.257 | 8.958×1010 | 0.495 |
| Li1+*x*V3O8 | 2.542×1022 | 4.655 | 3.112×1011 | 1.719 |
| LiMn2O4 | 5.220×1016 | 9.561×10−6 | 1.436×1011 | 0.793 |
| LiNi0.5Mn1.5O4 | 2.336×1024 | 4.279×102 | 1.145×1013 | 63.241 |
| LiFePO4 | 7.340×108 | 1.344×10−13 | 8.700×108 | 4.805×10−3 |
| Oxide  coating | Li4Ti5O12 | 5.922×108 | 3.265×10−16 | 8.510×108 | 4.700×10−3 |
| Li2ZrO3 | 2.438×109 | 1.344×10−15 | 9.383×108 | 5.182×10−3 |
| LiNbO3 | 6.626×108 | 3.653×10−16 | 8.537×108 | 4.714×10−3 |
| LiTaO3 | 6.884×108 | 3.795×10−16 | 1.034×109 | 5.709×10−3 |
| Sulfide  cathode | Li*x*TiS2 | / | / | 3.186×108 | 1.760×10−3 |
| Li*x*VS2 | 3.083×108 | 1.703×10−3 |
| Li*x*CrS2 | 2.831×108 | 1.564×10−3 |
| Li*x*MnS2 | 3.014×108 | 1.665×10−3 |
| Li*x*FeS2 | 3.640×108 | 2.010×10−3 |
| Li*x*CoS2 | 3.337×108 | 1.843×10−3 |
| Li*x*NiS2 | 3.160×108 | 1.745×10−3 |
| Li*x*CuS2 | 2.298×108 | 1.269×10−3 |
| Li*x*ZrS2 | 4.063×108 | 2.244×10−3 |
| Li*x*NbS2 | 3.254×108 | 1.797×10−3 |
| Li*x*MoS2 | 2.741×108 | 1.514×10−3 |
| Li*x*HfS2 | 3.257×108 | 1.799×10−3 |
| Li*x*TaS2 | 3.170×108 | 1.750×10−3 |
| Li*x*WS2 | 2.455×108 | 1.356×10−3 |
| Li2*x*V0.5Cr1.5S4 | 4.416×108 | 2.439×10−3 |
| Oxide  cathode | LiMnO2 | Li7La3Zr2O12 | 1.727×1010 | 3.163×10−12 | 1.178×1010 | 6.505×10−2 |
| LiFeO2 | 4.227×1010 | 7.742×10−12 | 1.270×1010 | 7.013×10−2 |
| LiCoO2 | 6.884×1011 | 1.261×10−10 | 1.045×1010 | 5.772×10−2 |
| LiNiO2 | 3.179×1010 | 5.822×10−12 | 1.037×1010 | 5.729×10−2 |
| NCM333 | 2.939×109 | 5.382×10−13 | 1.416×1010 | 7.821×10−2 |
| NCM523 | 6.941×109 | 1.271×10−12 | 1.508×1010 | 8.328×10−2 |
| NCM622 | 8.291×109 | 1.519×10−12 | 1.629×1010 | 8.994×10−2 |
| NCM811 | 8.619×109 | 1.579×10−12 | 1.738×1010 | 9.600×10−2 |
| Li2MnO3 | 6.684×1011 | 1.224×10−10 | 8.437×109 | 4.659×10−2 |
| Li1+*x*V3O8 | 6.286×1011 | 1.151×10−10 | 1.496×1010 | 8.260×10−2 |
| LiMn2O4 | 2.882×1010 | 5.278×10−12 | 9.083×109 | 5.016×10−2 |
| LiNi0.5Mn1.5O4 | 5.099×1011 | 9.339×10−11 | 1.464×1010 | 8.083×10−2 |
| LiFePO4 | 1.361×1010 | 2.493×10−12 | 1.614×1010 | 8.911×10−2 |
| Oxide  coating | Li4Ti5O12 | 1.098×1010 | 6.055×10−15 | 1.578×1010 | 8.716×10−2 |
| Li2ZrO3 | 4.521×1010 | 2.492×10−14 | 1.740×1010 | 9.611×10−2 |
| LiNbO3 | 1.229×1010 | 6.775×10−15 | 1.583×1010 | 8.744×10−2 |
| LiTaO3 | 1.277×1010 | 7.038×10−15 | 1.917×1010 | 0.106 |
| Sulfide  cathode | Li*x*TiS2 | / | / | 5.909×109 | 3.264×10−2 |
| Li*x*VS2 | 5.718×109 | 3.158×10−2 |
| Li*x*CrS2 | 5.251×109 | 2.900×10−2 |
| Li*x*MnS2 | 5.591×109 | 3.088×10−2 |
| Li*x*FeS2 | 6.752×109 | 3.729×10−2 |
| Li*x*CoS2 | 6.189×109 | 3.418×10−2 |
| Li*x*NiS2 | 5.861×109 | 3.237×10−2 |
| Li*x*CuS2 | 4.263×109 | 2.354×10−2 |
| Li*x*ZrS2 | 7.535×109 | 4.161×10−2 |
| Li*x*NbS2 | 6.034×109 | 3.333×10−2 |
| Li*x*MoS2 | 5.084×109 | 2.808×10−2 |
| Li*x*HfS2 | 6.041×109 | 3.336×10−2 |
| Li*x*TaS2 | 5.879×109 | 3.246×10−2 |
| Li*x*WS2 | 4.554×109 | 2.515×10−2 |
| Li2*x*V0.5Cr1.5S4 | 8.191×109 | 4.524×10−2 |
| Oxide  cathode | LiMnO2 | Li0.33La0.56TiO3 | 2.656×109 | 4.864×10−13 | 1.811×109 | 1.000×10−2 |
| LiFeO2 | 6.501×109 | 1.191×10−12 | 1.953×109 | 1.078×10−2 |
| LiCoO2 | 1.059×1011 | 1.939×10−11 | 1.607×109 | 8.876×10−3 |
| LiNiO2 | 4.888×109 | 8.953×10−13 | 1.595×109 | 8.810×10−3 |
| NCM333 | 4.519×108 | 8.277×10−14 | 2.178×109 | 1.203×10−2 |
| NCM523 | 1.067×109 | 1.955×10−13 | 2.319×109 | 1.281×10−2 |
| NCM622 | 1.275×109 | 2.335×10−13 | 2.504×109 | 1.383×10−2 |
| NCM811 | 1.325×109 | 2.428×10−13 | 2.673×109 | 1.476×10−2 |
| Li2MnO3 | 1.028×1011 | 1.883×10−11 | 1.297×109 | 7.165×10−3 |
| Li1+*x*V3O8 | 9.667×1010 | 1.770×10−11 | 2.300×109 | 1.270×10−2 |
| LiMn2O4 | 4.432×109 | 8.117×10−13 | 1.397×109 | 7.714×10−3 |
| LiNi0.5Mn1.5O4 | 7.841×1010 | 1.436×10−11 | 2.251×109 | 1.243×10−2 |
| LiFePO4 | 2.093×109 | 3.834×10−13 | 2.481×109 | 1.370×10−2 |
| Oxide  coating | Li4Ti5O12 | 1.689×109 | 9.311×10−16 | 2.427×109 | 1.340×10−2 |
| Li2ZrO3 | 6.953×109 | 3.833×10−15 | 2.676×109 | 1.478×10−2 |
| LiNbO3 | 1.890×109 | 1.042×10−15 | 2.435×109 | 1.345×10−2 |
| LiTaO3 | 1.964×109 | 1.082×10−15 | 2.949×109 | 1.628×10−2 |
| Sulfide  cathode | Li*x*TiS2 | / | / | 9.088×108 | 5.019×10−3 |
| Li*x*VS2 | 8.793×108 | 4.856×10−3 |
| Li*x*CrS2 | 8.076×108 | 4.460×10−3 |
| Li*x*MnS2 | 8.598×108 | 4.748×10−3 |
| Li*x*FeS2 | 1.038×109 | 5.734×10−3 |
| Li*x*CoS2 | 9.517×108 | 5.256×10−3 |
| Li*x*NiS2 | 9.014×108 | 4.978×10−3 |
| Li*x*CuS2 | 6.556×108 | 3.620×10−3 |
| Li*x*ZrS2 | 1.159×109 | 6.399×10−3 |
| Li*x*NbS2 | 9.280×108 | 5.125×10−3 |
| Li*x*MoS2 | 7.818×108 | 4.317×10−3 |
| Li*x*HfS2 | 9.290×108 | 5.131×10−3 |
| Li*x*TaS2 | 9.040×108 | 4.992×10−3 |
| Li*x*WS2 | 7.003×108 | 3.867×10−3 |
| Li2*x*V0.5Cr1.5S4 | 1.260×109 | 6.956×10−3 |
| Oxide  cathode | LiMnO2 | Li3OCl | 5.952×109 | 1.090×10−12 | 4.060×109 | 2.242×10−2 |
| LiFeO2 | 1.457×1010 | 2.668×10−12 | 4.377×109 | 2.417×10−2 |
| LiCoO2 | 2.373×1011 | 4.345×10−11 | 3.602×109 | 1.989×10−2 |
| LiNiO2 | 1.096×1010 | 2.007×10−12 | 3.575×109 | 1.975×10−2 |
| NCM333 | 1.013×109 | 1.855×10−13 | 4.881×109 | 2.696×10−2 |
| NCM523 | 2.392×109 | 4.381×10−13 | 5.198×109 | 2.870×10−2 |
| NCM622 | 2.858×109 | 5.234×10−13 | 5.613×109 | 3.100×10−2 |
| NCM811 | 2.971×109 | 5.441×10−13 | 5.991×109 | 3.309×10−2 |
| Li2MnO3 | 2.304×1011 | 4.219×10−11 | 2.908×109 | 1.606×10−2 |
| Li1+*x*V3O8 | 2.167×1011 | 3.968×10−11 | 5.155×109 | 2.847×10−2 |
| LiMn2O4 | 9.933×109 | 1.819×10−12 | 3.131×109 | 1.729×10−2 |
| LiNi0.5Mn1.5O4 | 1.757×1011 | 3.219×10−11 | 5.044×109 | 2.786×10−2 |
| LiFePO4 | 4.692×109 | 8.593×10−13 | 5.561×109 | 3.071×10−2 |
| Oxide  coating | Li4Ti5O12 | 3.786×109 | 2.087×10−15 | 5.440×109 | 3.004×10−2 |
| Li2ZrO3 | 1.558×1010 | 8.590×10−15 | 5.998×109 | 3.312×10−2 |
| LiNbO3 | 4.236×109 | 2.335×10−15 | 5.457×109 | 3.014×10−2 |
| LiTaO3 | 4.401×109 | 2.426×10−15 | 6.609×109 | 3.650×10−2 |
| Sulfide  cathode | Li*x*TiS2 | / | / | 2.037×109 | 1.125×10−2 |
| Li*x*VS2 | 1.971×109 | 1.088×10−2 |
| Li*x*CrS2 | 1.810×109 | 9.996×10−3 |
| Li*x*MnS2 | 1.927×109 | 1.064×10−2 |
| Li*x*FeS2 | 2.327×109 | 1.285×10−2 |
| Li*x*CoS2 | 2.133×109 | 1.178×10−2 |
| Li*x*NiS2 | 2.020×109 | 1.116×10−2 |
| Li*x*CuS2 | 1.469×109 | 8.114×10−3 |
| Li*x*ZrS2 | 2.597×109 | 1.434×10−2 |
| Li*x*NbS2 | 2.080×109 | 1.149×10−2 |
| Li*x*MoS2 | 1.752×109 | 9.677×10−3 |
| Li*x*HfS2 | 2.082×109 | 1.150×10−2 |
| Li*x*TaS2 | 2.026×109 | 1.119×10−2 |
| Li*x*WS2 | 1.570×109 | 8.668×10−3 |
| Li2*x*V0.5Cr1.5S4 | 2.823×109 | 1.559×10−2 |
| Oxide  cathode | LiMnO2 | LiTi2(PO4)3 | 3.272×109 | 5.993×10−13 | 2.232×109 | 1.233×10−2 |
| LiFeO2 | 8.011×109 | 1.467×10−12 | 2.406×109 | 1.329×10−2 |
| LiCoO2 | 1.304×1011 | 2.389×10−11 | 1.980×109 | 1.094×10−2 |
| LiNiO2 | 6.024×109 | 1.103×10−12 | 1.966×109 | 1.086×10−2 |
| NCM333 | 5.569×108 | 1.020×10−13 | 2.684×109 | 1.482×10−2 |
| NCM523 | 1.315×109 | 2.409×10−13 | 2.858×109 | 1.578×10−2 |
| NCM622 | 1.571×109 | 2.878×10−13 | 3.086×109 | 1.704×10−2 |
| NCM811 | 1.633×109 | 2.991×10−13 | 3.294×109 | 1.819×10−2 |
| Li2MnO3 | 1.267×1011 | 2.320×10−11 | 1.599×109 | 8.830×10−2 |
| Li1+*x*V3O8 | 1.191×1011 | 2.182×10−11 | 2.834×109 | 1.565×10−2 |
| LiMn2O4 | 5.461×109 | 1.000×10−12 | 1.721×109 | 9.506×10−3 |
| LiNi0.5Mn1.5O4 | 9.663×1010 | 1.770×10−11 | 2.773×109 | 1.532×10−2 |
| LiFePO4 | 2.580×109 | 4.725×10−13 | 3.058×109 | 1.689×10−2 |
| Oxide  coating | Li4Ti5O12 | 2.081×109 | 1.147×10−15 | 2.991×109 | 1.652×10−2 |
| Li2ZrO3 | 8.567×109 | 4.723×10−15 | 3.298×109 | 1.821×10−2 |
| LiNbO3 | 2.329×109 | 1.284×10−15 | 3.000×109 | 1.657×10−2 |
| LiTaO3 | 2.420×109 | 1.334×10−15 | 3.633×109 | 2.007×10−2 |
| Sulfide  cathode | Li*x*TiS2 | / | / | 1.120×109 | 6.184×10−3 |
| Li*x*VS2 | 1.084×109 | 5.984×10−3 |
| Li*x*CrS2 | 9.951×108 | 5.496×10−3 |
| Li*x*MnS2 | 1.059×109 | 5.851×10−3 |
| Li*x*FeS2 | 1.279×109 | 7.066×10−3 |
| Li*x*CoS2 | 1.173×109 | 6.476×10−3 |
| Li*x*NiS2 | 1.111×109 | 6.134×10−3 |
| Li*x*CuS2 | 8.078×108 | 4.461×10−3 |
| Li*x*ZrS2 | 1.428×109 | 7.886×10−3 |
| Li*x*NbS2 | 1.144×109 | 6.315×10−3 |
| Li*x*MoS2 | 9.634×108 | 5.320×10−3 |
| Li*x*HfS2 | 1.145×109 | 6.322×10−3 |
| Li*x*TaS2 | 1.114×109 | 6.152×10−3 |
| Li*x*WS2 | 8.629×108 | 4.766×10−3 |
| Li2*x*V0.5Cr1.5S4 | 1.552×109 | 8.572×10−3 |
| Oxide  cathode | LiMnO2 | Li2PO2N | 5.248×1010 | 9.611×10−12 | 3.731×1010 | 0.206 |
| LiFeO2 | 7.066×1010 | 1.294×10−11 | 3.917×1010 | 0.216 |
| LiCoO2 | 8.942×1010 | 1.638×10−11 | 3.441×1010 | 0.190 |
| LiNiO2 | 6.374×1010 | 1.167×10−11 | 3.558×1010 | 0.197 |
| NCM333 | 1.213×1010 | 2.222×10−12 | 4.543×1010 | 0.251 |
| NCM523 | 3.410×1010 | 6.244×10−12 | 4.448×1010 | 0.246 |
| NCM622 | 3.019×1010 | 5.529×10−12 | 5.305×1010 | 0.293 |
| NCM811 | 3.079×1010 | 5.639×10−12 | 4.941×1010 | 0.273 |
| Li2MnO3 | 9.349×1010 | 1.712×10−11 | 3.141×1010 | 0.174 |
| Li1+*x*V3O8 | 1.103×1011 | 2.019×10−11 | 3.869×1010 | 0.214 |
| LiMn2O4 | 5.926×1010 | 1.085×10−11 | 3.348×1010 | 0.185 |
| LiNi0.5Mn1.5O4 | 9.561×1010 | 1.751×10−11 | 4.298×1010 | 0.237 |
| LiFePO4 | 7.203×1010 | 1.319×10−11 | 6.373×1010 | 0.352 |
| Oxide  coating | Li4Ti5O12 | 4.644×1010 | 2.560×10−14 | 9.924×1010 | 0.548 |
| Li2ZrO3 | 5.427×1010 | 2.992×10−14 | 7.716×1010 | 0.426 |
| LiNbO3 | 4.396×1010 | 2.423×10−14 | 8.496×1010 | 0.469 |
| LiTaO3 | 5.390×1010 | 2.971×10−14 | 4.154×1010 | 0.229 |
| Sulfide  cathode | Li*x*TiS2 | / | / | 2.487×1010 | 0.137 |
| Li*x*VS2 | 2.279×1010 | 0.126 |
| Li*x*CrS2 | 2.105×1010 | 0.116 |
| Li*x*MnS2 | 2.379×1010 | 0.131 |
| Li*x*FeS2 | 2.823×1010 | 0.156 |
| Li*x*CoS2 | 3.049×1010 | 0.168 |
| Li*x*NiS2 | 2.516×1010 | 0.139 |
| Li*x*CuS2 | 2.614×1010 | 0.144 |
| Li*x*ZrS2 | 2.436×1010 | 0.135 |
| Li*x*NbS2 | 6.074×1010 | 0.335 |
| Li*x*MoS2 | 5.101×1010 | 0.282 |
| Li*x*HfS2 | 2.253×1010 | 0.124 |
| Li*x*TaS2 | 2.380×1010 | 0.131 |
| Li*x*WS2 | 1.788×1010 | 9.875×10−2 |
| Li2*x*V0.5Cr1.5S4 | 3.810×1010 | 0.210 |
| Oxide  cathode | LiMnO2 | Li3YCl6 | 3.014×109 | 5.519×10−13 | 2.056×109 | 1.135×10−2 |
| LiFeO2 | 7.377×109 | 1.351×10−12 | 2.216×109 | 1.224×10−2 |
| LiCoO2 | 1.201×1011 | 2.200×10−11 | 1.824×109 | 1.007×10−2 |
| LiNiO2 | 5.547×109 | 1.016×10−12 | 1.810×109 | 9.998×10−3 |
| NCM333 | 5.129×108 | 9.393×10−14 | 2.472×109 | 1.365×10−2 |
| NCM523 | 1.211×109 | 2.218×10−13 | 2.632×109 | 1.453×10−2 |
| NCM622 | 1.447×109 | 2.650×10−13 | 2.842×109 | 1.570×10−2 |
| NCM811 | 1.504×109 | 2.755×10−13 | 3.034×109 | 1.675×10−2 |
| Li2MnO3 | 1.166×1011 | 2.136×10−11 | 1.472×109 | 8.131×10−3 |
| Li1+*x*V3O8 | 1.097×1011 | 2.009×10−11 | 2.610×109 | 1.442×10−2 |
| LiMn2O4 | 5.029×109 | 9.211×10−13 | 1.585×109 | 8.754×10−3 |
| LiNi0.5Mn1.5O4 | 8.899×1010 | 1.630×10−11 | 2.554×109 | 1.411×10−2 |
| LiFePO4 | 2.376×109 | 4.351×10−13 | 2.816×109 | 1.555×10−2 |
| Oxide  coating | Li4Ti5O12 | 1.917×109 | 1.057×10−15 | 2.754×109 | 1.521×10−2 |
| Li2ZrO3 | 7.890×109 | 4.349×10−15 | 3.037×109 | 1.677×10−2 |
| LiNbO3 | 2.145×109 | 1.182×10−15 | 2.763×109 | 1.526×10−2 |
| LiTaO3 | 2.228×109 | 1.228×10−15 | 3.346×109 | 1.848×10−2 |
| Sulfide  cathode | Li*x*TiS2 | / | / | 1.031×109 | 5.695×10−3 |
| Li*x*VS2 | 9.979×108 | 5.511×10−3 |
| Li*x*CrS2 | 9.165×108 | 5.061×10−3 |
| Li*x*MnS2 | 9.757×108 | 5.388×10−3 |
| Li*x*FeS2 | 1.178×109 | 6.507×10−3 |
| Li*x*CoS2 | 1.080×109 | 5.964×10−3 |
| Li*x*NiS2 | 1.023×109 | 5.649×10−3 |
| Li*x*CuS2 | 7.440×108 | 4.109×10−3 |
| Li*x*ZrS2 | 1.315×109 | 7.262×10−3 |
| Li*x*NbS2 | 1.053×109 | 5.816×10−3 |
| Li*x*MoS2 | 8.872×108 | 4.900×10−3 |
| Li*x*HfS2 | 1.054×109 | 5.822×10−3 |
| Li*x*TaS2 | 1.026×109 | 5.666×10−3 |
| Li*x*WS2 | 7.947×108 | 4.389×10−3 |
| Li2*x*V0.5Cr1.5S4 | 1.429×109 | 7.894×10−3 |
| Oxide  cathode | LiMnO2 | Li3InCl6 | 2.306×109 | 4.224×10−13 | 1.573×109 | 8.687×10−3 |
| LiFeO2 | 5.645×109 | 1.034×10−12 | 1.696×109 | 9.366×10−3 |
| LiCoO2 | 9.193×1010 | 1.684×10−11 | 1.396×109 | 7.708×10−3 |
| LiNiO2 | 4.245×109 | 7.775×10−13 | 1.385×109 | 7.651×10−3 |
| NCM333 | 3.925×108 | 7.188×10−14 | 1.891×109 | 1.045×10−2 |
| NCM523 | 9.269×108 | 1.698×10−13 | 2.014×109 | 1.112×10−2 |
| NCM622 | 1.107×109 | 2.028×10−13 | 2.175×109 | 1.201×10−2 |
| NCM811 | 1.151×109 | 2.108×10−13 | 2.321×109 | 1.282×10−2 |
| Li2MnO3 | 8.926×1010 | 1.635×10−11 | 1.127×109 | 6.223×10−3 |
| Li1+*x*V3O8 | 8.395×1010 | 1.538×10−11 | 1.997×109 | 1.103×10−2 |
| LiMn2O4 | 3.849×109 | 7.049×10−13 | 1.213×109 | 6.699×10−3 |
| LiNi0.5Mn1.5O4 | 6.810×1010 | 1.247×10−11 | 1.955×109 | 1.079×10−2 |
| LiFePO4 | 1.818×109 | 3.330×10−13 | 2.155×109 | 1.190×10−2 |
| Oxide  coating | Li4Ti5O12 | 1.467×109 | 8.086×10−16 | 2.108×109 | 1.164×10−2 |
| Li2ZrO3 | 6.038×109 | 3.328×10−15 | 2.324×109 | 1.283×10−2 |
| LiNbO3 | 1.641×109 | 9.048×10−16 | 2.114×109 | 1.168×10−2 |
| LiTaO3 | 1.705×109 | 9.400×10−16 | 2.561×109 | 1.414×10−2 |
| Sulfide  cathode | Li*x*TiS2 | / | / | 7.892×109 | 4.358×10−3 |
| Li*x*VS2 | 7.636×109 | 4.217×10−3 |
| Li*x*CrS2 | 7.013×108 | 3.873×10−3 |
| Li*x*MnS2 | 7.466×108 | 4.123×10−3 |
| Li*x*FeS2 | 9.017×108 | 4.980×10−3 |
| Li*x*CoS2 | 8.265×108 | 4.564×10−3 |
| Li*x*NiS2 | 7.828×108 | 4.323×10−3 |
| Li*x*CuS2 | 5.693×108 | 3.144×10−3 |
| Li*x*ZrS2 | 1.006×109 | 5.558×10−3 |
| Li*x*NbS2 | 8.059×108 | 4.451×10−3 |
| Li*x*MoS2 | 6.789×108 | 3.749×10−3 |
| Li*x*HfS2 | 8.068×108 | 4.456×10−3 |
| Li*x*TaS2 | 7.851×108 | 4.336×10−3 |
| Li*x*WS2 | 6.081×108 | 3.359×10−3 |
| Li2*x*V0.5Cr1.5S4 | 1.094×109 | 6.041×10−3 |

1. **Code manual for interfacial resistance calculations based on ligand-field and space-charge layer model**

**2.1 Introduction**

**Illustrating (electro)chemical-/electric-potential profiles in the SCL at the open circuit.** The contact between the cathode and the SE causes the internal carriers (ions or electrons) to be driven from SE region with higher chemical potential to the cathode region1. Given the electronic insulation and ion conduction properties of the SE, a locally electrically non-neutral region, *viz.*, an SCL, resulting from the migration of uncompensated charges across the boundary is formed at the cathode/SE interface2. At this point, an interfacial electric-potential difference exists between the cathode and the SE. The electrochemical potential (, *i* is the carrier) is adopted to describe the carrier migration behavior in the electrically non-neutral region, which consists of the chemical potential () and the electric-potential ()3:

where is the charge number of carrier (*e.g.*, = 1 for Li+) and is the Faraday constant. The , and of the carriers in the bulk (*i.e.*, the region far from the interface) of cathode, SE, and anode, as well as at their interfaces, are shown in Fig. 1a. is the partial molar Gibbs free energy, ignoring electrostatic contributions. is the line integral of the electric field along a path from a reference point (often at an infinite distance from the interface) to a given position. Only the redistribution of ions at the interface is considered because of the insulative nature of SE. When the lithium ions in cathode, SE, and anode reach equilibrium through redistribution, their electrochemical potential becomes constant:

where is the vertical distance from the *k* position (nm, *k* = 1, 2, …) in SE to the cathode/SE interface junction (*k* = 0), so the initial is equal to 0 nm. Considering that the chemical potential () depends on the lithium-ionconcentration (), we link the change in the interfacial electric-potential to the one in the lithium-ionconcentration. By substituting Eq. 1 and Eq. 2 into Eq. 3, the Boltzmann distribution of the lithium-ion concentration can be obtained, as shown in Eq. 4 and Eq. 5:

where is the standard chemical potential, is the molar standard concentration, R is the molar gas constant, is Boltzmann constant, and *T* is Kelvin temperature. and are the lithium-ionconcentrations at and on the interface. is the interfacial electric-potential difference at *k* position (, Fig. 1b).

The remaining problem is how to obtain the interfacial electric-potential. The upper limit of at the cathode/SE interface is the , *i.e.*, . Formally, one may separate the chemical potential of Li into the electrochemical potentials of the electrons and ions (), while the electronic contribution is generally assumed to play a dominating role4. Thus, can be expressed as the difference in the Li chemical potential between cathode and anode (), which is dominated by the electronic electrochemical potential difference between cathode and anode ():

Notably, is dominated by the Fermi level () in solid materials5. One can obtain the Fermi level difference between cathode and anode to express the open circuit voltage, which is also the upper limit of interfacial electric-potential at the cathode/SE interface. However, calculating the Fermi level using conventional Density Functional Theory (DFT) based on the bulk structure is unsuitable for the interfacial structure because of the structural deformation and atomic movement at the interface. Therefore, it is necessary to focus on the model for mapping the interfacial Fermi levels and the corresponding resistance properties.

**Constructing a modified crystal-field splitting strength (MCFSS) descriptor.** The Fermi level of the cathode is determined using the crystal-field splitting strength (Fig. S1), which can be divided into two terms, *viz.*, transition-metal (TM)-d splitting coefficient (*n*) and TM-d orbital splitting strength (). Our previous work6 shows that the strength of can be described by: , where is the charge on the ligand, is the average of fourth power of the core-electron distance, and *L* is the TM-ligand bond length. By comparing the calculated data with the theoretical formula, the ionic radius can be used instead of for different central metal ions7. Thus, the crystal-field splitting strength can be expressed as follows:

Based on this, a MCFSS descriptor for evaluating the upper limit of cathode/SE interfacial electric-potential difference is constructed:

where is the bandgap of the system. for metal or semiconductor cathodes because electrons are accepted by their valence bands during SCL formations, whereas for insulator cathodes, , electrons are received by their conduction bands. Considering that the lithium-ions in the SE are depleted, the interfacial electric-potential difference is always positive (Eq. 5). Then, |MCFSS| is introduced into the SCL model as the initial interfacial electric-potential difference () to further simulate the dynamic evolutions of the ion concentration (), electric field intensity (), and electric-potential () in different regions of the interface. The calculation process for the MCFSS is illustrated in Fig. 1c.

**Proposing ligand-field and space-charge layer integrated numerical procedure.** Poisson-equation is the basic equation that describes the carrier redistribution in space, which leads to the formation of SCL. In view of the fact that the carrier distribution at the interface is determined by the chemical potential gradient from bulk to interface, the one-dimensional Poisson-equation (Eq. 9) is usually used to analyze the carrier rearrangement in this direction. The one-dimensional treatment of Poisson-equation is proved to be effective for studying the proton distribution at the electrolyte side in oxide fuel cell8and the oxygen-ion distribution in photocatalytic materials9. In this case, the one-dimensional Poisson-equation is expressed as follows:

where is the permittivity. The local net charge density is a function of the lithium-ion concentration, and can be written as:

Since the entire system is electrically neutral when the lithium-ion are not rearranged, the depletion at the interface inevitably leads to a negative net charge in SCL (). Introducing electric field intensity () is necessary to solve Poisson-equation numerically. is related to and its numerical solution is proposed by Maier10:

Assuming that the bulk material is electrically neutral, *viz*., and , the relation between electric field intensity and interfacial electric-potential can be obtained by integrating Eq. 12.

At this point, it is assumed that there is an intermediate process, that is, the depleted lithium ions in SE are all gathered on cathode surface (that is, *k*=0), so the charge density of SCL can be obtained by calculating the electric field intensity at the interface ().

The accumulated charge of the whole SCL () is calculated and divided into equal number of calculation steps (). The corresponding intervals can then be easily determined using the local charge density.

The interfacial electric-potential at the new coordinate () is calculated using Taylor series to the third order.

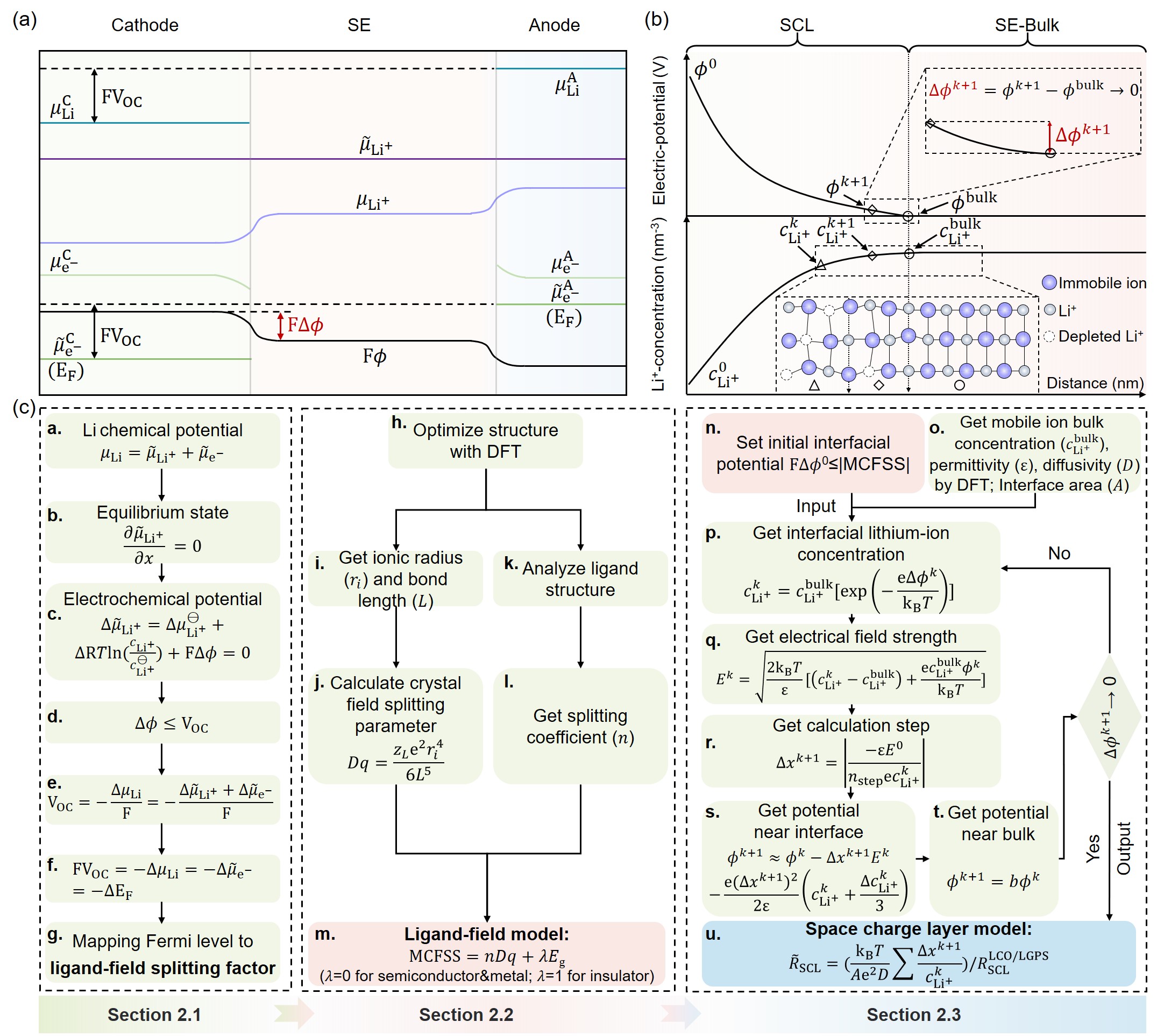
can be expressed as follows:

If (the initial calculation), then . Because of the gentle change trend of the electric-potential near the bulk, the charge density decreases slowly, leading to rather large intervals of *x* and thus to an inaccurately calculated SCL range. For this purpose, a is defined, which is the electric-potential when the lithium ion concentration at the interface () differs marginally from (here chosen as the factor 10−7 according to previous literature10). Note that the is also the value of , so the *x* interval problem is solved while ensuring the continuity of the electric-potential profiles within SCL:

Subsequently, the factor is defined to determine the . is a parameter introduced to distinguish the impact of structural distortion and electronic structure on interfacial resistance between different interface systems (Table S5).

If the interfacial electric-potential at position meets convergence criteria (), we then calculate the interfacial resistance resulting from SCL (), and further propose a normalized SCL resistance () based on the calculated of representative LiCoO2/Li10GeP2S12 (LCO/LGPS) interface to facilitate the observation of the relative resistance trend of different interface systems:

where is the lithium-ion conductivity, is the lithium-ion diffusivity, and is the surface area. Otherwise, the first step is returned, and the lithium-ion concentration at the following position () is solved. The numerical calculation process for is shown in Fig. 1c. The numerical calculation procedure of integrating the ligand field and space-charge layer models is implemented in a computational platform for battery materials11.



**Figure 1**. (a) Electric (), chemical (), and electrochemical () potential profiles for Li+, e–, and neutral Li in ASSB under open circuit voltage (). is dominated by the Fermi level ()22. The superscripts C and A represent the cathode and anode, respectively. (b) Schematic diagram of the variations of electric-potential () and lithium-ion concentration () with distances () in SCL. (c) The workflow for calculating the of cathode/coating and SE interfaces by the proposed ligand-field and space-charge layer integrated procedure. The splitting parameter (*Dq*) and splitting coefficient (*n*) are obtained using ligand-field model (see Code Availability). Then, the lithium-ion concentration (), electric field intensity (), calculation step (), and electric-potential () at the interface are iterated. If convergence criteria () is met, the is further calculated.

**2.2 Hardware and software requirements**

Hardware requirements:

* Processor: Intel or AMD dual-core, main frequency above 1GHz
* Memory: 4G

Software requirements:

* Operating system: Windows 7 and above
* Python 3.8
* Numpy 1.21.0
* Scipy 1.7.0
* Pandas 1.3.0

**2.3 Input file**

The input files that need to be prepared include “input\_parameter.py” and “input\_mcfss.py”.

**Cathode or coating setting in “input\_parameter.py”**

The “input\_parameter.py” already includes the existing oxide cathode (oca), oxide coating (oco), and sulfide cathode (sca). If additional cathode or coating types need to be added, a new function can be generated by copying the existing functions (def oca(), def oco(), and def oca()) in this module (the name after def needs to be assigned by users, and **the values in the function do not need to be assigned separately, they can be all assigned to 1**).

**Table 2.** Properties of SE that need to be defined by the user (taking Li7La3Zr2O12 as an example).

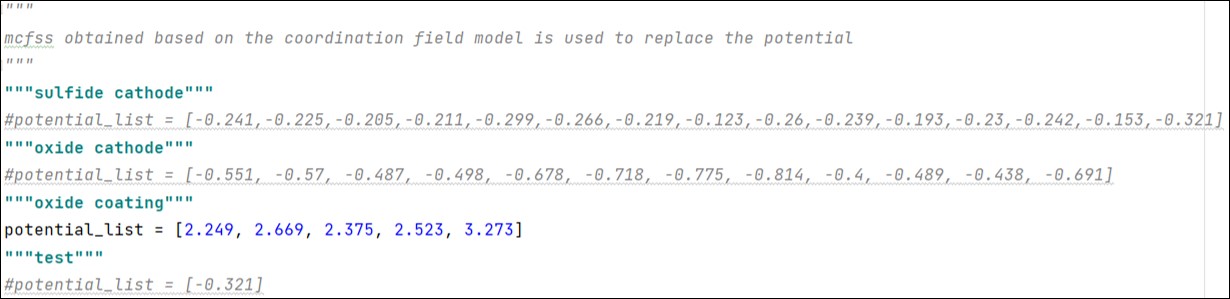
|  |  |  |
| --- | --- | --- |
| **Parameter** | **Value** | **Description** |
| z\_i | 1 | The charge number of carrier |
| c\_bulk | 10.085 | The carrier concentration (nm‒3) |
| surface | 1 | The cross-sectional area of interface (nm2) |
| permittivity | 5.743 | The relative permittivity of SE |
| diffusivity | 4E-9 | The lithium-ion diffusivity of SE (cm2 s‒1) |
| electric\_potential | 0 | The bulk electric-potential (V) |

**SE setting in input\_parameter.py**

If user wants to add a new SE, they can copy and generate a new function according to the existing functions, such as def li7la3zr2o12(). User needs to define the properties of SE, as shown in Table 2.

* **z\_i:** The charge number of the carrier, such as +1 for lithium-ion and −1 for electron.
* **c\_bulk:** The carrier concentration, which can be obtained through the Nernst-Einstein equation (). It is necessary to obtain the diffusivity and conductivity of carrier by experiment or DFT calculation.
* **permittivity:** The relative permittivity of the SE, which is calculated by DFT.
* **diffusivity:** The diffusivity of lithium-ion in SE, which can be obtained by DFT calculation or directly from experiments.
* **surface:** The cross-sectional area of the interface, which is set to 1 nm2 by default.
* **electric\_potential:** The electric-potential of SE, which is set to 0 V by default.

Finally, enter the cathode (or coating) type (*e.g.*, “oca”), the name of the SE (*e.g.*, "li7la3zr2o12"), and the type of SE (*e.g.*, “oxide”) at the top of the module into “cathode”, “se”, and “se\_type” respectively.



**Figure 2.** The MCFSS value of the cathode or coating that needs to be calculated by the user.

**Electric-potential setting in “input\_mcfss.py”**

The “input\_mcfss.py” file already contains MCFSS for 31 types of cathodes or coatings. If the user wants to **calculate the MCFSS of other cathodes or coatings**, it is needed to enter the “**MOELD-LLF**” file under the previous file. **Use the MOELD-LLF procedure to parse the POSCAR file and output the corresponding ligand-field splitting coefficient (*n*)**. The specific principle and usage details are also included in this folder. According to the Eq. 7-8, after obtaining the ligand-field splitting coefficient, the MCFSS of the material can be calculated by combining the ionic radius and the bond length provided in POSCAR file. **Enter the MCFSS** of corresponding material type (such as “oxide cathode”, “oxide coating”, “sulfide cathode”, or user-defined type, which is defined in the same way that functions are defined in “input\_parameter.py”) in the “**potential\_list**”.

**2.4 Running the code**

This procedure was written on the PyCharm interpreter. It is recommended to use this interpreter to run the procedure.

(a) Prepare “input\_parameter.py” and “input\_mcfss.py”.

(b) Click on the “\_\_init\_\_.py” module and click on the “Run” button under it or use the shortcut keys “Ctrl+F5”.

**2.5 Output File**

**Table 3.** Taking Li7La3Zr2O12 as electrolyte and oxides as cathodes, the initial electric-potentials (phi\_0) and the calculated SCL resistance (resistance\_scl) at different interfaces are presented.

|  |  |  |
| --- | --- | --- |
| **index** | **phi\_0 (V)** | **resistance\_scl (Ω)** |
| 1 | ‒0.551 | 1.178×1010 |
| 2 | ‒0.57 | 1.270×1010 |
| 3 | ‒0.487 | 1.045×1010 |
| 4 | ‒0.498 | 1.037×1010 |
| 5 | ‒0.678 | 1.416×1010 |
| 6 | ‒0.718 | 1.508×1010 |
| 7 | ‒0.775 | 1.629×1010 |
| 8 | ‒0.814 | 1.738×1010 |
| 9 | ‒0.4 | 8.437×109 |
| 10 | ‒0.489 | 1.496×1010 |
| 11 | ‒0.551 | 1.178×1010 |
| 12 | ‒0.57 | 1.270×1010 |

The “**scl\_resistance.csv**” file is generated in the current folder, which includes the calculated interface number, the initial interfacial electric-potentials, and the interfacial resistances between the cathodes (or coatings) and the SEs. For example, the Table 3 shows the output values of the oxide cathode/Li7La3Zr2O12 SE.

* **index**: The calculated interface number.
* **phi\_0**: The initial interfacial electric-potential, which is described by MCFSS in “input\_mcfss”.
* **scl\_resistance**: The space-charge layer resistance (). The normalized space-charge layer resistance () shown in the results is obtained by dividing it by the space-charge layer resistance of LiCoO2/Li10GeP2S12 ().

**2.6 Example**

If you want to make further use of the ILFSCL-IRNCP code, please follow:

(a) Preparing the properties of the selected cathode, coating, and SE materials in “input\_parameter.py” and “input\_mcfss.py”.

(b) Running the “\_\_init\_\_.py” module and obtain the interfacial resistance between the selected cathode (or coating) and SE.

You will get results that contain the raw data.

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