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

**V 1.0**

2023-6-2

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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-state electrolyte (SSE), surface area (*A*), permittivity (), diffusivity (*D*), and bulk electric-potential (). “input\_mcfss.py” is used to assign the required electric-potential parameters. This corresponds to the MCFSS (the detailed description and obtaining method are showed in **2.1** and **2.3** respectively) or band values used in the manuscript to replace the interfacial electric-potential difference.

**1.2 Data**

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

The “input\_mcfss.py” file contains the electric-potential parameters of 31 cathode and coating materials, from 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 SSE materials (mentioned in **1.1**), from 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 cathode, coating, and SSE in the “input\_parameter.py” and “input\_mcfss.py” files. In the end, the output file “scl\_resistance.csv”, contains the interfacial resistance and the SSE, 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)/SSE interfaces.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Type | Cathode or coating | Solid state electrolyte | (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. **The manual for calculation code of interfacial resistance based on ligand-field and space-charge-layer**

**2.1 Introduction**

**Illustrating (electro)chemical-potential (/) and electric-potential () profiles in SCL at open circuit.** The contact between cathode and SSE causes the internal carriers (ions or electrons) to be driven from the high chemical potential SSE region to the low chemical potential cathode region1. Considering the electronic insulation and ion conduction properties of SSE, a locally non-electrical region resulting from migration of uncompensated charges across the boundary2, *viz.*, space-charge-layer (SCL) can be formed at the cathode/SSE interface. At this point, an interfacial electric-potential exists between the cathode and the SSE. The electrochemical potential () is adopted to describe carrier migration behavior in non-electrically neutral regions, which consists of chemical potential () and electric-potential ():

where *i* is carriers (Li+ or e–), is the charge number of carriers (*e.g.*, = 1 for Li+) and is the Faraday constant. The relationship between the , and of the carriers in the bulk (*i.e.*, the region far from the interface) of cathode, SSE, and anode, as well as at their interfaces are shown in Fig. 1a. The chemical potential 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 infinite distance from the system) to a given position. In addition, only the redistribution of ions at the interface is considered due to the insulation of SSE and the fact that its ionic conductivity is several orders of magnitude higher than its electronic conductivity. When the lithium-ion in the cathode, SSE, and anode reach equilibrium through the redistribution, the electrochemical potential of lithium-ion becomes constant:

where is the vertical distance from the *k* position (*k* = 1, 2 …) in SSE to the cathode/SSE 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 of interfacial electric-potential to the change of the lithium-ionconcentration. By substituting Eq. 1 and Eq. 2 into Eq. 3, the Boltzmann distribution of 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 molar gas constant, is Boltzmann constant, *T* is Kelvin temperature. and are the lithium-ionconcentration at and on the interface. is the interfacial electric-potential difference at *k* position (, Fig. 1b).

The remaining problem is to obtain the interfacial electric-potential. The threshold of potential difference at the cathode/SSE interface is the open circuit voltage (), *i.e.*, . Formally, one may separate the Li chemical potential into the electrochemical potentials of the electrons and the ions (), while the electronic contribution is generally assumed to play a dominating role3. Thus, can be expressed by the difference in Li chemical potential between cathode and anode (), which is dominated by the electrochemical potentials difference of electrons () between the cathode and anode:

Notably, is dominated by the Fermi level4. One can obtain the Fermi level difference between cathode and anode to express the open circuit voltage, which is also the threshold of interfacial electric-potential at the cathode/SSE interface. However, the calculation of Fermi level by conventional DFT based on the bulk structure is not suitable for the interfacial structure because of the structural deformation and atomic movement at the interface. Therefore, it is necessary turn attention to the model of mapping the interfacial Fermi levels and corresponding resistance properties.

**Proposing a ligand-field descriptor (MCFSS) to evaluate the threshold of .** The Fermi level of cathode is determined by crystal field splitting strength (CFSS), which can be divided into two aspects, *viz.*, TM-d splitting coefficient (*n*) and TM-d orbitals splitting strength (). Our previous work proposed that the strength of can be described by5: , where is the charge on the ligand, is the fourth power of the average core-electron distance, and *R* is the M-ligand bond length. By comparing the calculated data with theoretical formula, when the central ion is the same period, the ion radius can be used instead of 6. Thus, CFSS can be expressed as follows:

Based on this, an interfacial ligand-field descriptor for evaluating the upper limit of cathode/SSE interfacial electric-potential difference is proposed:

where is the band gap of system. for metal or semiconductor cathodes because electrons are accepted by their valence band during SCL formation, while for insulator cathodes, because electrons are received by their valence band in this case. Considering that the lithium-ion in the SSE 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 evolution of ion concentration (), electric field intensity () and potential () in different regions of the interface. The calculation process of MCFSS is shown in Fig. 1c.

**Quantifying interfacial normalized SCL resistance ().** Poisson-equation is the basic equation describing the charge distribution in space, *e.g.*, the redistribution of charges which lead to the formation of SCL. To simplify the model, we only consider the Poisson-equation in the one-dimensional state, which is expressed as follows

where is the permittivity. The local net charge density is a function of the lithium-ion concentration, one can write:

In view of the fact that the entire system is electrically neutral when the lithium-ions are not rearranged, the depletion of lithium-ions at the interface inevitably leads to a negative net charge at the interface (). It is necessary to introduce electric field intensity () to solve Poisson-equation numerically. is related to , and its numerical solution is proposed by Maier7:

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-ion in SSE all gather on the surface of the cathode (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 in calculation steps () equally large quantities. The corresponding intervals can then be easily determined using the local charge density.

The interfacial electric-potential at the new coordinate is calculated according to a Taylor approximation of degree three.

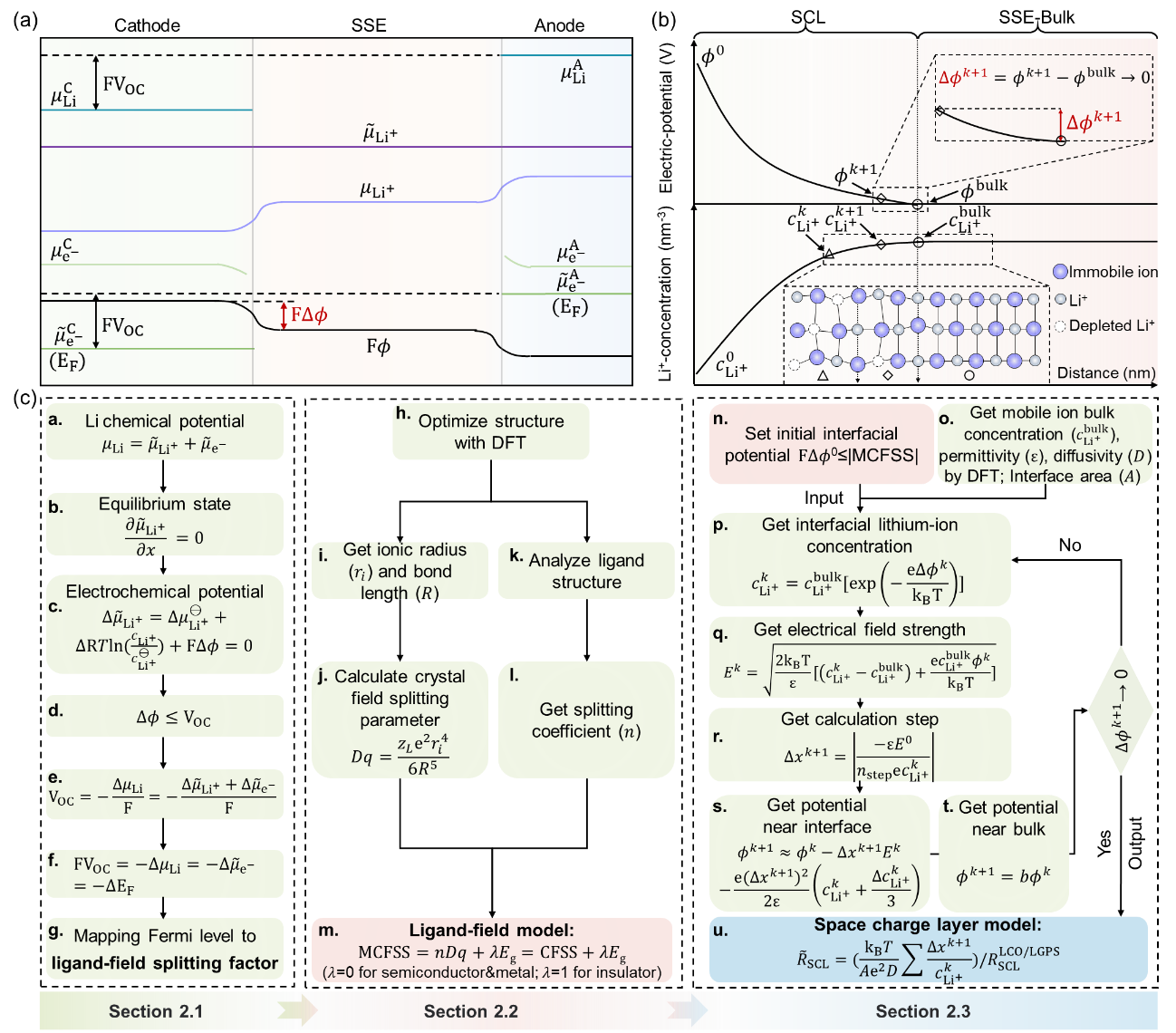
can be expressed as follows:

If *k*=0 (the initial calculation), then . Notably, when the change of electric-potential is far away from the interface junction, it is easy for Eq. 17 to make errors when describing electric-potential due to excessive change, so it is necessary to describe potential change in another manner. For this purpose, an electric-potential is defined. It is the value of , for which the concentration of the lithium-ion () differs only marginally from its bulk value (the factor is set to 10−7 according to previous literature7):

where a 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.

If the interfacial electric-potential at position to meet 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 diffusivity and *A* is the surface area. Otherwise, the first step is returned and the lithium-ion concentration at the next position () is solved. The numerical calculation process of is shown in Fig. 1c. Procedures of numerical calculation method of integrated ligand-field and space-charge-layer model were implemented in the computational platform for battery materials8.



**Figure 1**. (a) Electric (), chemical (), and electrochemical () potential profiles for Li+, e–, and neutral Li in ASSLMB under open circuit voltage (). is dominated by the electronic Fermi level ()4. The superscript C and A represent the cathode and anode, respectively. The upper limit of the interfacial electric-potential difference between cathode and SSE () is . (b) Schematic diagram of the variation of electric-potential () and lithium-ion concentration () with distance () in SCL. The convergence condition is satisfied when approaches 0. (c) The workflow for calculating the  between cathodes/coatings and SSEs by combining ligand-field and SCL models. is dominated by the electron electrochemical potential (, *viz*., ). The splitting parameter (*Dq*) and splitting coefficient (*n*) are obtained by our ligand-field model (as available at 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 fully assigned 1**).

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

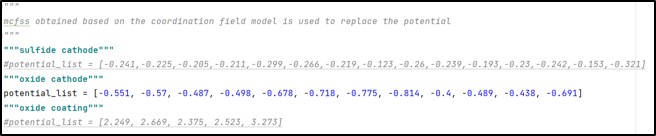
**Table 2.** Properties of SSE that require user definition (take Li7La3Zr2O12, for example).

|  |  |  |
| --- | --- | --- |
| **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 SSE |
| diffusivity | 4E-9 | The diffusivity of SSE (cm2 s‒1) |
| voltage | 0 | The bulk electric-potential (V) |

If user wants to add a new SSE, which also copy and generate a new function according to the existing functions, such as def li7la3zr2o12(). User needs to define the properties of SSE, 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 SSE, which is calculated by DFT.
* **diffusivity:** The diffusivity of lithium-ion in SSE, 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.
* **voltage:** The electric-potential of SSE, which is set to 0 V by default.

Finally, enter the cathode (or coating) type (e.g. “oca”), the name of the SSE (e.g. "li7la3zr2o12"), and the type of SSE (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 31 types of MCFSS for cathodes or coatings. If the user wants to **calculate the MCFSS of other cathodes or coatings**, he needs 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. After obtaining the ligand-field splitting coefficient, the MCFSS of the corresponding material is calculated combined with the required ionic radius and the bond length in the POSCAR file according to the Eq. 7-8. **Enter the MCFSS** of corresponding material type (such as “oxide cathode”, “oxide coating”, “sulfide cathode”, or user-defined type, with the similar defined method referring to the method of defining the function 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.** The number of interfaces calculated, the initial electric-potential, and the space-charge-layer-resistance. The SSE is Li7La3Zr2O12 and the cathode is oxide cathode.

|  |  |  |
| --- | --- | --- |
| **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 number of interfaces calculated, the initial interfacial electric-potential, and the interfacial resistance between the cathode (or coating) and the SSE. For example, the Table 3 shows the output values of the oxide cathode/Li7La3Zr2O12.

* **index**: The number of interfaces calculated.
* **phi\_0**: The initial interfacial electric-potential, which is replaced by MCFSS in “input\_mcfss”.
* **scl\_resistance**: The space-charge-layer resistance (). To further calculate the normalized space-charge-layer resistance (), divide 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 required cathode, coating, and SSE materials in “input\_parameter.py” and “input\_mcfss.py”.

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

You will retain the results containing the raw data.

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