

OPINCHARGE presentation

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Opincharge consortium



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Project Overview



OPINCHARGE



WP5/Top challenges

- 1. <u>Meso-scale modelling of interphases</u>
 - SEI transport, reaction processes, and structure
 - Continuum Models and kinetic Monte Carlo models (KMC)
- 2. <u>Homogenized degradation modelling</u>
 - Automated analysis of EIS spectra with ML algorithms
- 3. <u>Correlation of interface properties with electronic/ionic transport</u>
 - Redox-Probe experiments (see next slide)
- 4. <u>Electrochemical validation at full cell level</u>
 - Polarization, EIS, cycling and CV to validate models
- 5. <u>Reference electrode design</u> and continuous electrode monitoring
 - Integrate a 3D porous reference electrode in pouch cell



WP5/Preliminary experimental results



[1] Steinrück, Chem. Phys. 154, 174703 (2021) [2] Strmcnik et al., Nat Catal 1, 255 (2018).



WP5/Preliminary modelling results

Silicon Voltage Hysteresis

Chemo-Mechanical Continuum Model in core-shell geometry



Voltage:
$$U = -\frac{\mu_{\text{Li}}}{F} = U_0 + \frac{\nu_{\text{Li}}}{3F\lambda_{\text{ch}}^3}\mathbf{P}$$
: **F**

Visco-elastoplastic shell behavior explains OCV and GITT Hysteresis



[1] Köbbing et al., Adv. Funct. Mater. 34, 2308818 (2024)



Conclusions/Perspectives

- Tools are being developed: other "Battery 2030+" projects interested in using them/collaborating?
- Links on our project webpage <u>https://www.opincharge.eu/project/</u>; interested in doing the same? + social media?