

Supporting Information

The simulation of interface characteristics and charge transfer dynamics for layered electrodes using cascade capacitance in supercapacitors by COMSOL software

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1.Parameters of activated carbon as negative electrode

Property	Variable	Value	Unit	Property group
Electrical conductivity	σ_{iso} ; $\sigma_{mii} = \sigma_{iso}$, $\sigma_{mij} = 0$	32.4[S/m]	S/m	Basic
Electrolyte conductivity	$\sigma_{mal,iso}$; $\sigma_{mal,ii} = \sigma_{mal,iso}$, $\sigma_{mal,ij} = 0$	80[S/m]	S/m	Electrolyte conductivity
Diffusion coefficient	D_{iso} ; $D_{ii} = D_{iso}$, $D_{ij} = 0$	$3.9e-14[m^2/s]$	m^2/s	Basic
Density	ρ	$2260[kg/m^3]$	kg/m^3	Basic
Equilibrium potential	Eeq	Eeq_int1(soc)	V	Equilibrium potential
Temperature derivative of equilibrium potential	dEeqdT	0[V/K]	V/K	Equilibrium potential
Reference concentration	cEeqref	def.csmax	mol/m^3	Equilibrium potential
Maximum electrode state of charge	socmax	elpot.Eeq_inv(E_min)	1	Operational electrode state of charge
Minimum electrode state of charge	socmin	elpot.Eeq_inv(E_max)	1	Operational electrode state of charge
Maximum operational potential	E_max	4.2[V]	V	Operational electrode state of charge
Minimum operational potential	E_min	0[V]	V	Operational electrode state of charge
Equilibrium concentration	csEq	def.csmax*elpot.Eeq_inv(V)	mol/m^3	Equilibrium concentration

2.Parameters of KOH solution as electrolyte

Property	Variable	Value	Unit	Property group
Electrolyte conductivity	$\sigma_{mal,iso}$; $\sigma_{mal,ii} = \sigma_{mal,iso}$, $\sigma_{mal,ij} = 0$	$(A*M+B*M^2+C*M*T_K+D*M/T_K+E*M^3+F*M^2*T_K^2)*1[S/cm]$	S/m	Electrolyte conductivity
Diffusion coefficient	D_{iso} ; $D_{ii} = D_{iso}$, $D_{ij} = 0$	$3.75e-9[m^2/s]$	m^2/s	Basic
Density	ρ	$(A_{rho}(T_{degC})^2+B_{rho}(T_{degC})^3+M_{reg}+C_{rho}(T_{degC}))*1[kg/m^3]$	kg/m^3	Basic
Transport number	transpNum	0.22	1	Species properties
Activity dependence	fcl	2	1	Species properties

3.Parameters of graphene oxide as positive electrode

Property	Variable	Value	Unit	Property group
Electrical conductivity	σ_{iso} ; $\sigma_{mii} = \sigma_{iso}$, $\sigma_{mij} = 0$	1000[S/m]	S/m	Basic
Electrolyte conductivity	$\sigma_{mal,iso}$; $\sigma_{mal,ii} = \sigma_{mal,iso}$, $\sigma_{mal,ij} = 0$	100[S/m]	S/m	Electrolyte conductivity
Young's modulus	E	E_int(c/csmax)	Pa	Basic
Poisson's ratio	ν	$\nu_{int}(c/csmax)$	1	Basic
Diffusion coefficient	D_{iso} ; $D_{ii} = D_{iso}$, $D_{ij} = 0$	$1.4523e-13*exp(68025.7/8.314*(1/(T_{ref}/1[K])-1/(T/1[K]))) [m^2/s]$	m^2/s	Basic
Thermal conductivity	k_{iso} ; $k_{ii} = k_{iso}$, $k_{ij} = 0$	$1[W/(m*K)]$	$W/(m*K)$	Basic
Heat capacity at constant pressure	Cp	750[J/(kg*K)]	J/(kg*K)	Basic
Density	ρ	2300[kg/m^3]	kg/m^3	Basic
Equilibrium potential	Eeq	Eeq_int1(soc)+dEeqdT_int1(soc)*(T-298[K])	V	Equilibrium potential
Temperature derivative of equilibrium potential	dEeqdT	dEeqdT_int1(soc)	V/K	Equilibrium potential
Reference concentration	cEeqref	def.csmax	mol/m^3	Equilibrium potential
Maximum electrode state of charge	socmax	elpot.Eeq_inv(E_min)	1	Operational electrode state of charge
Minimum electrode state of charge	socmin	elpot.Eeq_inv(E_max)	1	Operational electrode state of charge
Maximum operational potential	E_max	4.2[V]	V	Operational electrode state of charge
Minimum operational potential	E_min	0[V]	V	Operational electrode state of charge
Volumetric strain	dvolt	dvoltDSOL(c/def.csmax)	1	Intercalation strain
Equilibrium concentration	csEq	def.csmax*elpot.Eeq_inv(V)	mol/m^3	Equilibrium concentration

4.Parameters of ZnMn₂O₄ as positive electrode

Property	Variable	Value	Unit	Property group
<input checked="" type="checkbox"/> Electrical conductivity	σ_{iso} ; $\sigma_{\text{mai}} = \sigma_{\text{iso}}$, $\sigma_{\text{maj}} = 0$	1000[S/m]	S/m	Basic
<input checked="" type="checkbox"/> Electrolyte conductivity	$\sigma_{\text{mal}}_{\text{iso}}$; $\sigma_{\text{mali}} = \sigma_{\text{mal}}_{\text{iso}}$, $\sigma_{\text{malj}} = 0$	100[S/m]	S/m	Electrolyte conductivity
Young's modulus	E	E_int(c/c _{smax})	Pa	Basic
Poisson's ratio	nu	nu_int(c/c _{smax})	1	Basic
Diffusion coefficient	D _{iso} ; D _{ii} = D _{iso} , D _{ij} = 0	$1.4523 \times 10^{-13} \exp(68025.7/8.314 \cdot (1/(T_{\text{ref}}/1[\text{K}]) - 1/(T/1[\text{K}]))) [\text{m}^2/\text{s}]$	m ² /s	Basic
Thermal conductivity	k _{iso} ; k _{ii} = k _{iso} , k _{ij} = 0	1[W/(m·K)]	W/(m·K)	Basic
Heat capacity at constant pressure	C _p	750J/(kg·K)	J/(kg·K)	Basic
Density	rho	2300[kg/m ³]	kg/m ³	Basic
Equilibrium potential	E _{eq}	E _{eq_int1} (soc)+dE _{eqdT_int1} (soc)*(T-298[K])	V	Equilibrium potential
Temperature derivative of equilibrium potential	dE _{eqdT}	dE _{eqdT_int1} (soc)	V/K	Equilibrium potential
Reference concentration	c _{Eqref}	def.c _{smax}	mol/m ³	Equilibrium potential
Maximum electrode state of charge	soc _{max}	elpot.E _{eq_inv} (E _{min})	1	Operational electrode state of charge
Minimum electrode state of charge	soc _{min}	elpot.E _{eq_inv} (E _{max})	1	Operational electrode state of charge
Maximum operational potential	E _{max}	4.2[V]	V	Operational electrode state of charge
Minimum operational potential	E _{min}	0[V]	V	Operational electrode state of charge
Volumetric strain	dvol	dVOLdSOL(c/def.c _{smax})	1	Intercalation strain
Equilibrium concentration	cs _{Eq}	def.c _{smax} *elpot.E _{eq_inv} (V)	mol/m ³	Equilibrium concentration