

Description of Additional Supplementary Files

File Name: Supplementary Data 1

Description: Calculation data of solvation structure of BE electrolyte. (Gromacs) (Fig 1d)

File Name: Supplementary Data 2

Description: Calculation data of solvation structure of DDSLE electrolyte. (Gromacs) (Fig 1e)

File Name: Supplementary Data 3

Description: Calculation data of molecular orbital energy of DDSLE electrolyte solvation clusters. (Gaussian) (Fig 1h-SI 5)

File Name: Supplementary Data 4

Description: Calculation data of NFS surface electron density distribution. (Vasp) (Fig 2b)

File Name: Supplementary Data 5

Description: Calculation data of NFS/DDSLE interface model. (Vasp) (Fig 2c)

File Name: Supplementary Data 6

Description: Calculation data of adsorption energy of each component of the electrolyte at the NFS positive electrode interface (Vasp) and calculation data of molecular orbital energy of each component of the electrolyte. (Gaussian) (Fig 2d-SI 9)

File Name: Supplementary Data 7

Description: Calculation data of adsorption energy of each component of the electrolyte at the Na metal interface (Vasp) and calculation data of molecular orbital energy of each component of the electrolyte. (Gaussian) (Fig 5a)

File Name: Supplementary Data 8

Description: Calculation data of solvation structure of DE electrolyte. (Gromacs) (SI 21b)