GEMS

MLZ
Heinz Maier-Leibnitz Zentrum

Study of Ionic Liquids and Deep Eutectic Solvents at a Solid Electrode

Molecular Dynamics Simulations and Neutron Reflectometry

Dr. Nebojša Zec

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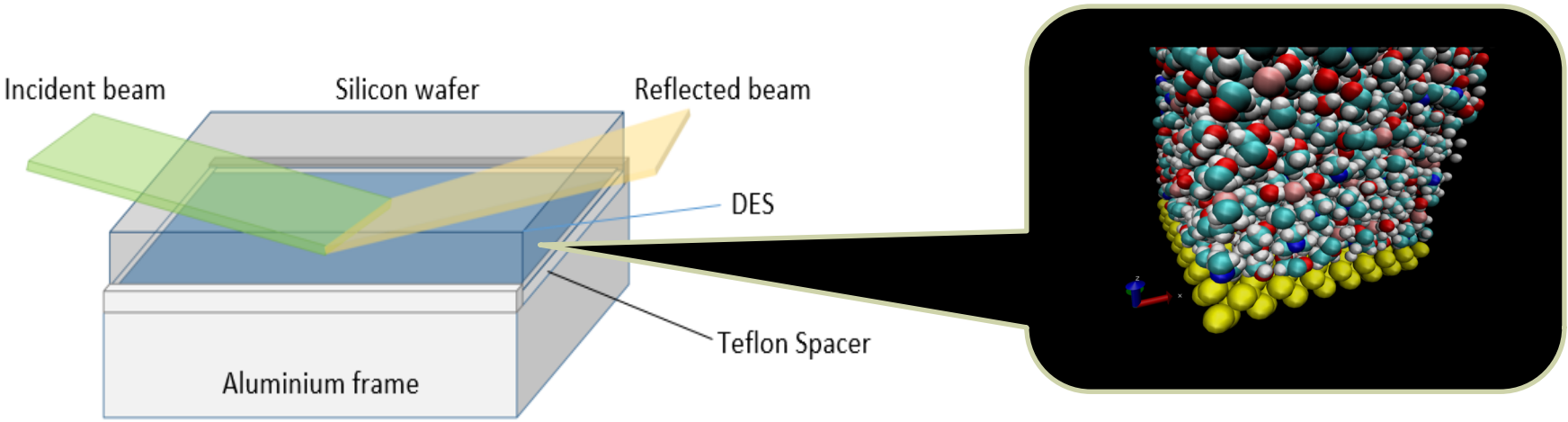
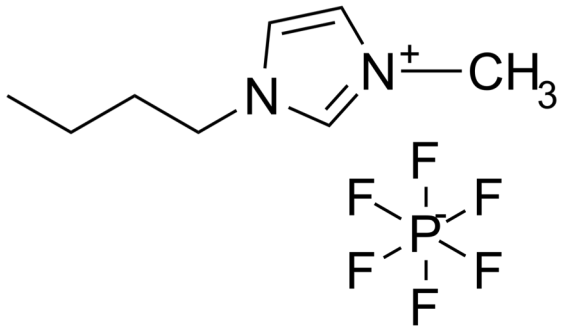


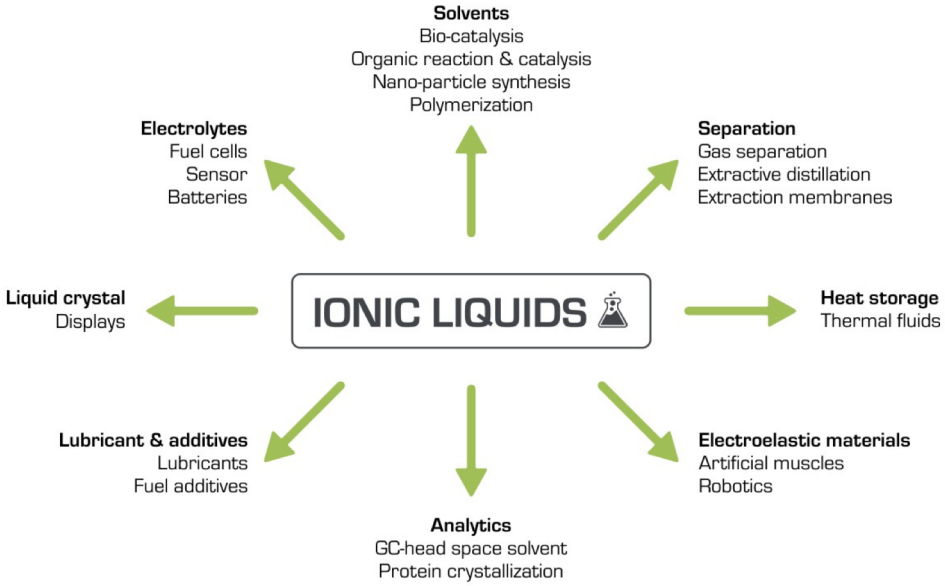
JÜLICH Forschungszentrum

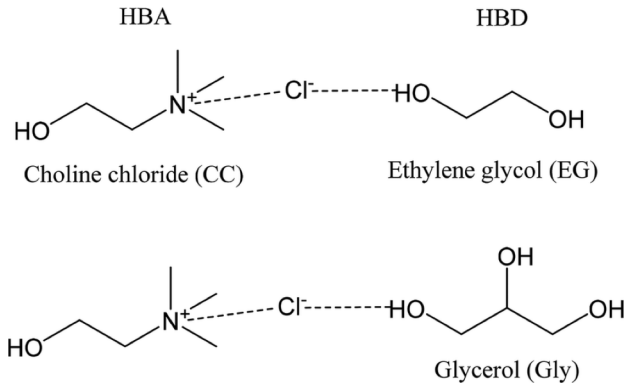
Helmholtz-Zentrum Geesthacht
Zentrum für Material- und Küstenforschung

Technical University of Munich

Ionic Liquids and Deep Eutectic Solvents







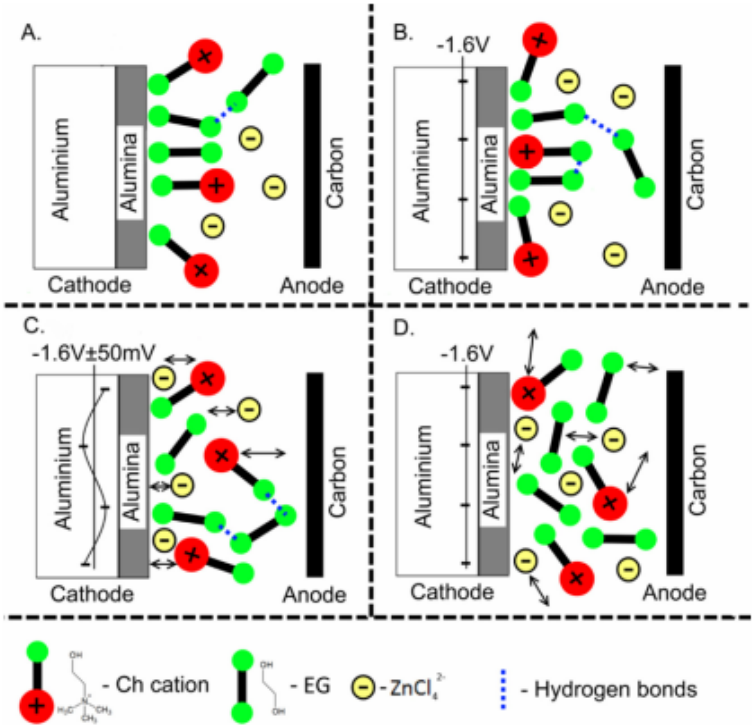
Contents lists available at ScienceDirect

Electrochimica Acta

journal homepage: www.elsevier.com/locate/electacta

Electrochemical deposition of zinc from deep eutectic solvent on barrier alumina layers

M. Starykevich [a], A.N. Salak [a], D.K. Ivanou [b,c], A.D. Lisenkov [a], M.L. Zheludkevich [a,d], M.G.S. Ferreira [a,*]



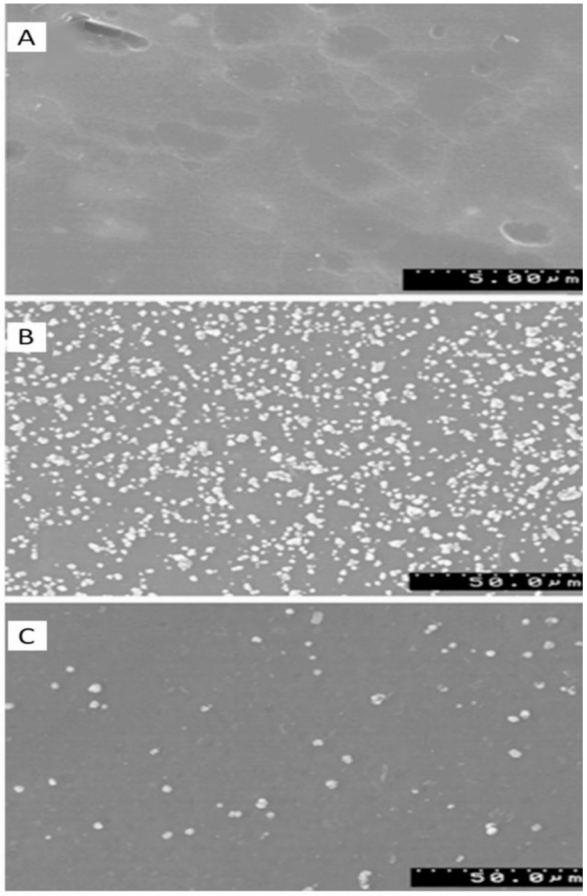
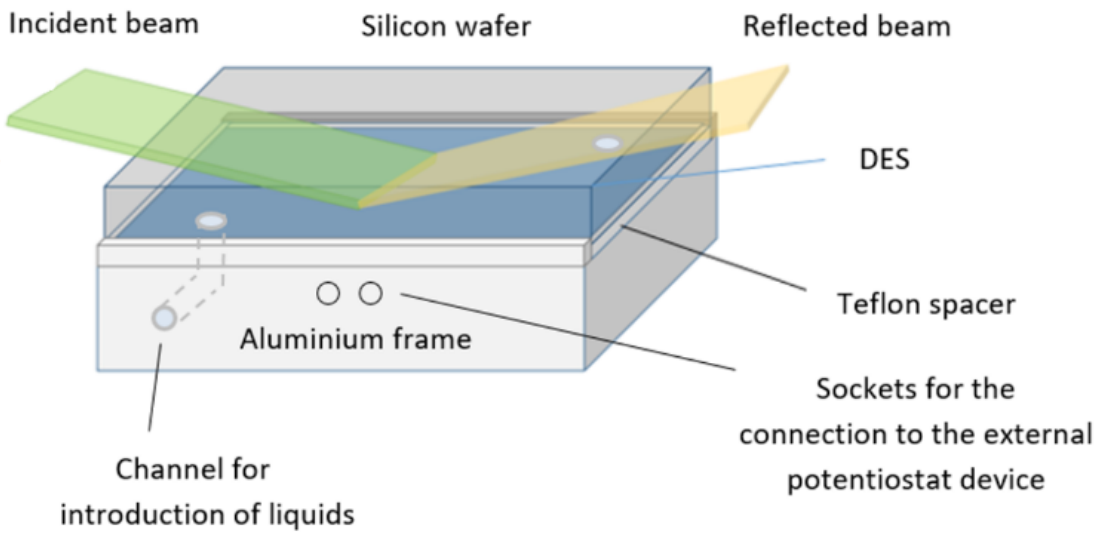


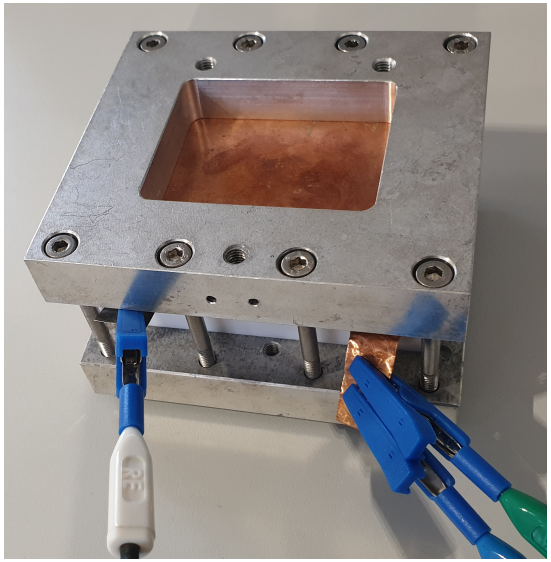
Fig. 4. Stable layer structured of choline/ethylene glycol on the electrode surface in absence of potential (A) and at constant potential (PS mode) (B). Destabilization of the layer as a result of application of an AC-PS mode (C) or/and increasing temperature (D).


JJ X-RAY
GAMRY

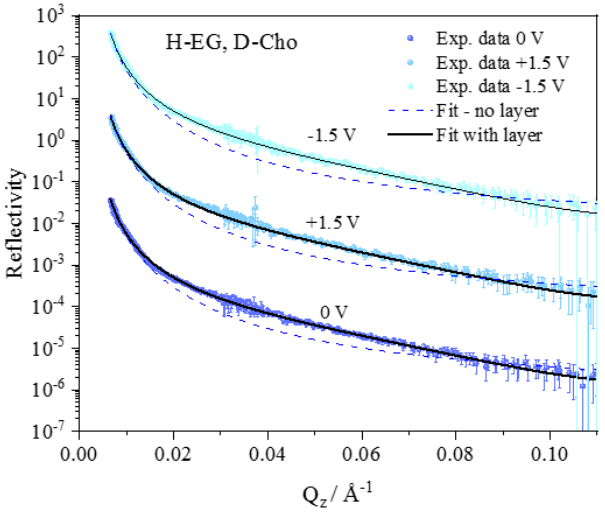
REFSANS


Incident beam
Silicon wafer
Reflected beam
DES
Teflon spacer
Aluminium frame
Sockets for the connection to the external potentiostat device
Channel for introduction of liquids

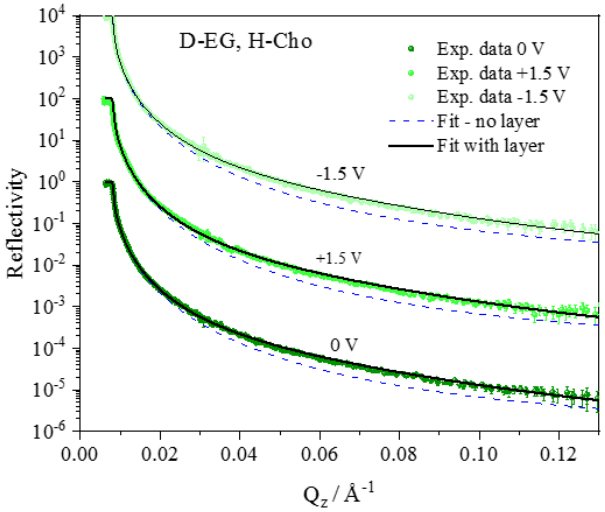

JJ X-RAY



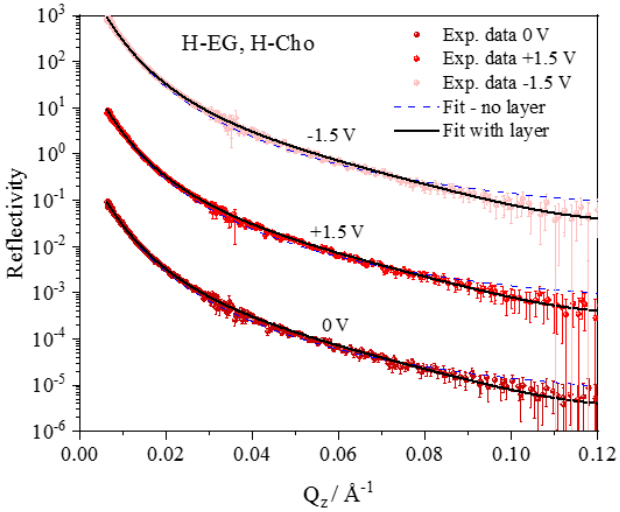
H-ethylene glycol
D-choline chloride



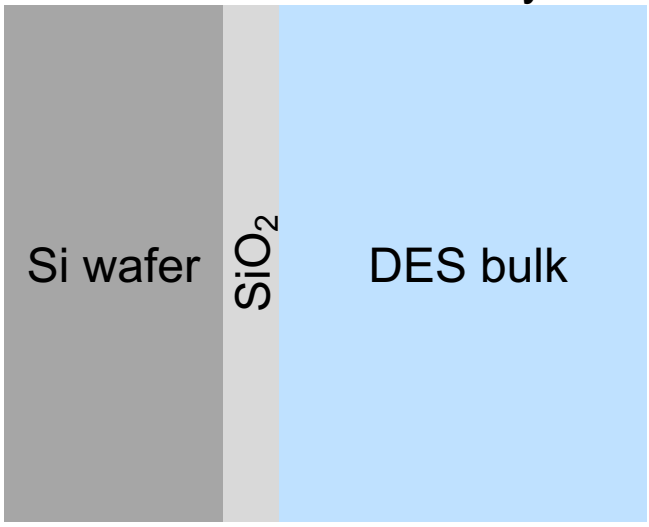
D-ethylene glycol
H-choline chloride



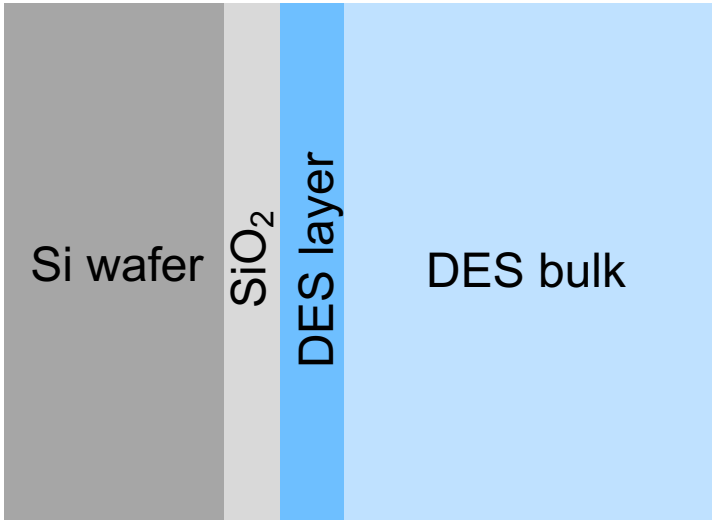
H-ethylene glycol
H-choline chloride



Model 1 – no DES layer

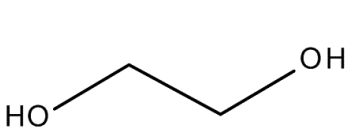


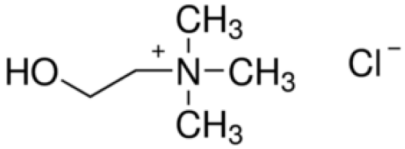
Model 2 – with the layer

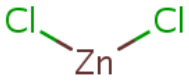


Ethaline

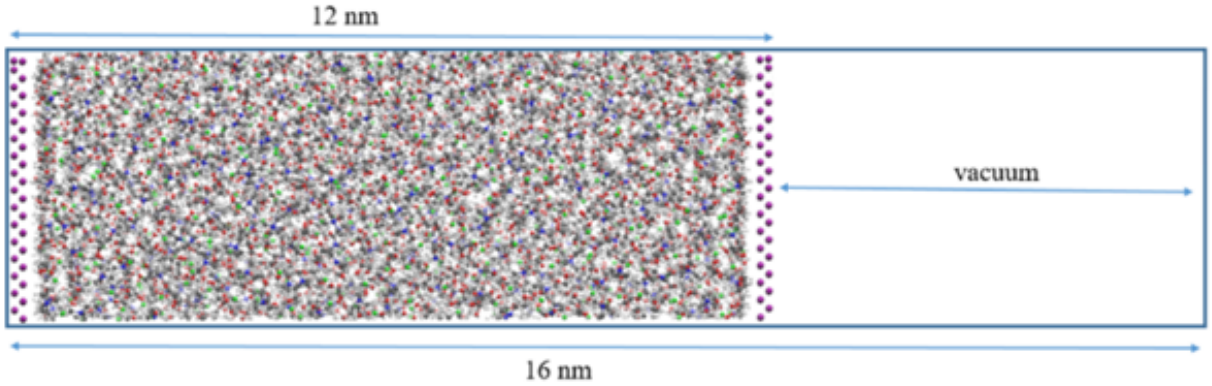
Ethylene Glycol 1024 + Choline Chloride 512 + Zinc Chloride 20

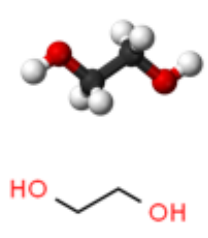




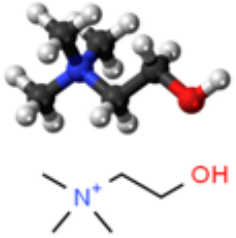


GROMACS
FAST. FLEXIBLE. FREE.



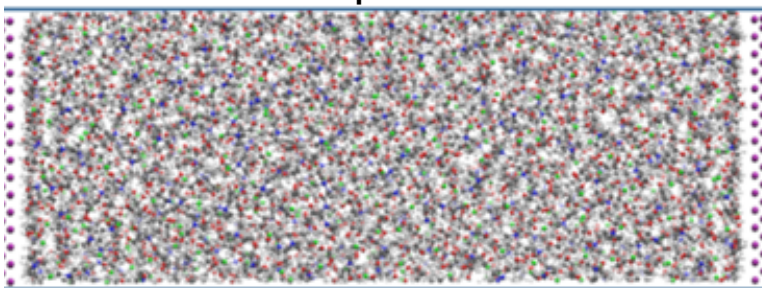


Ethylene glycol

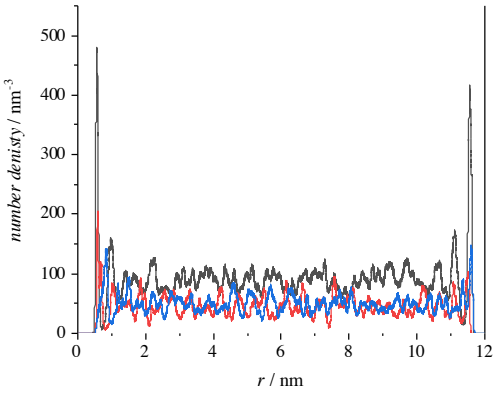


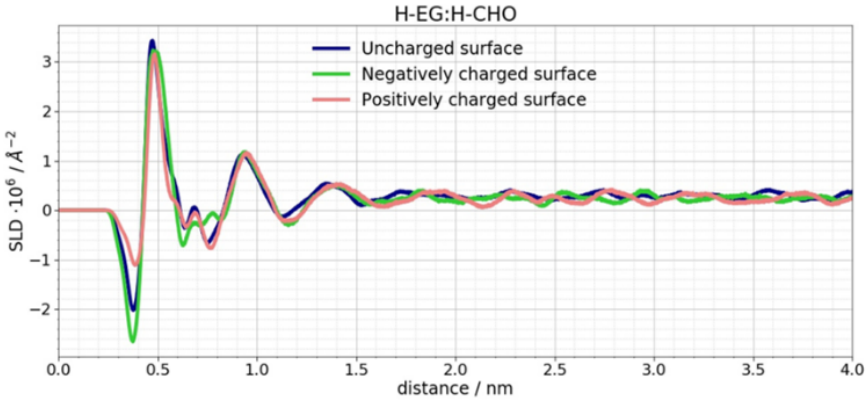
Choline

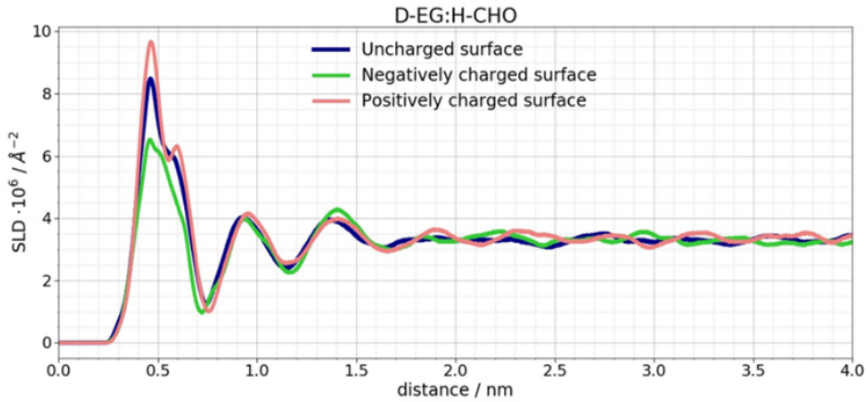
MD Simulations
12 replicas

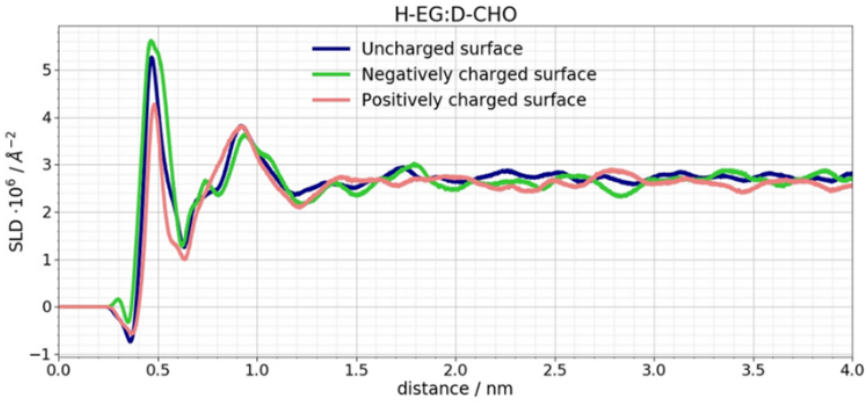


TRAVIS
+ In house Python scripts

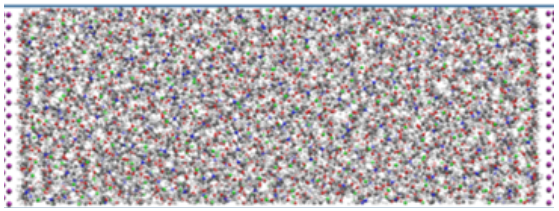


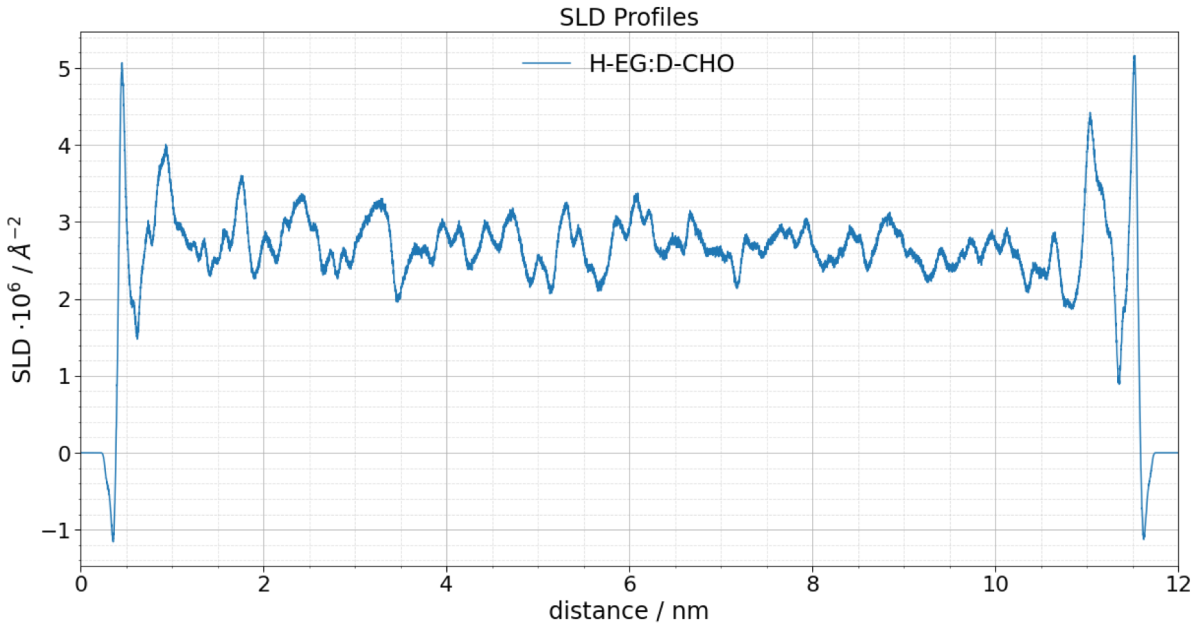




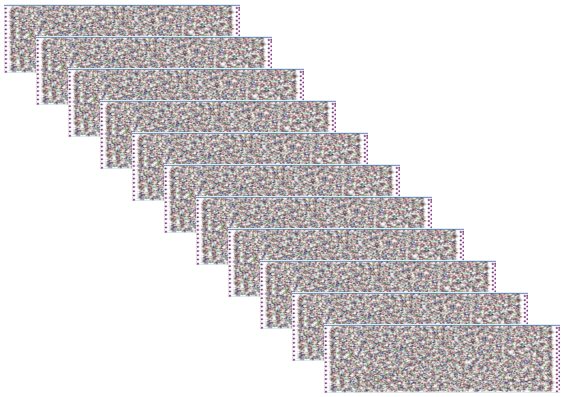


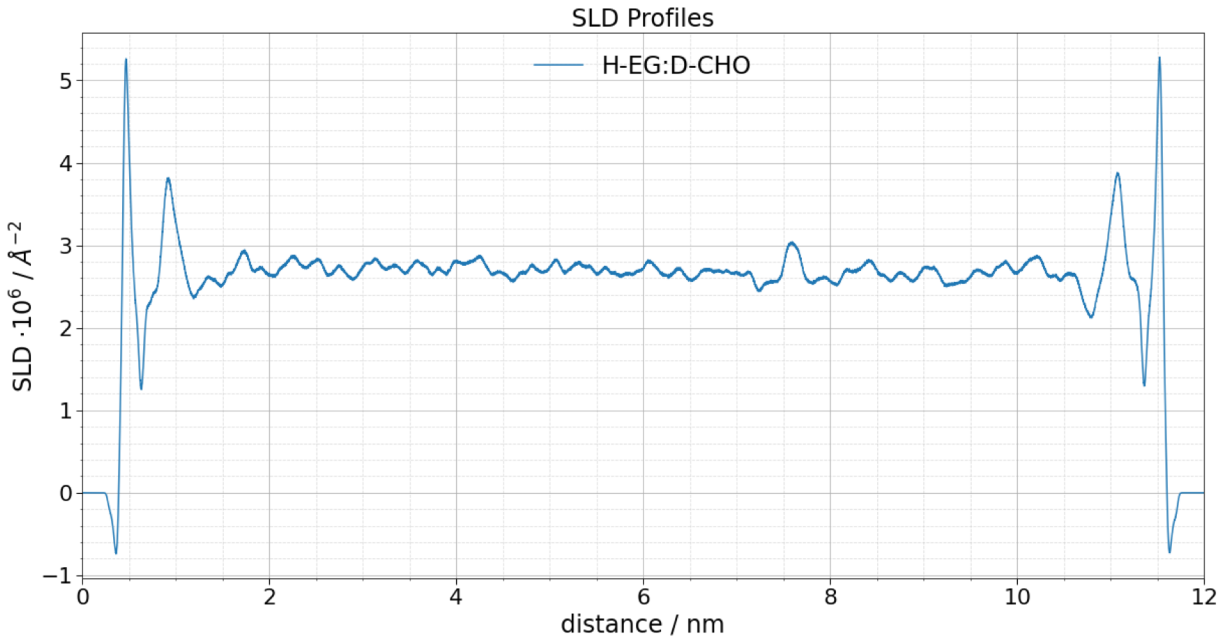
1 simulation (100 ns)

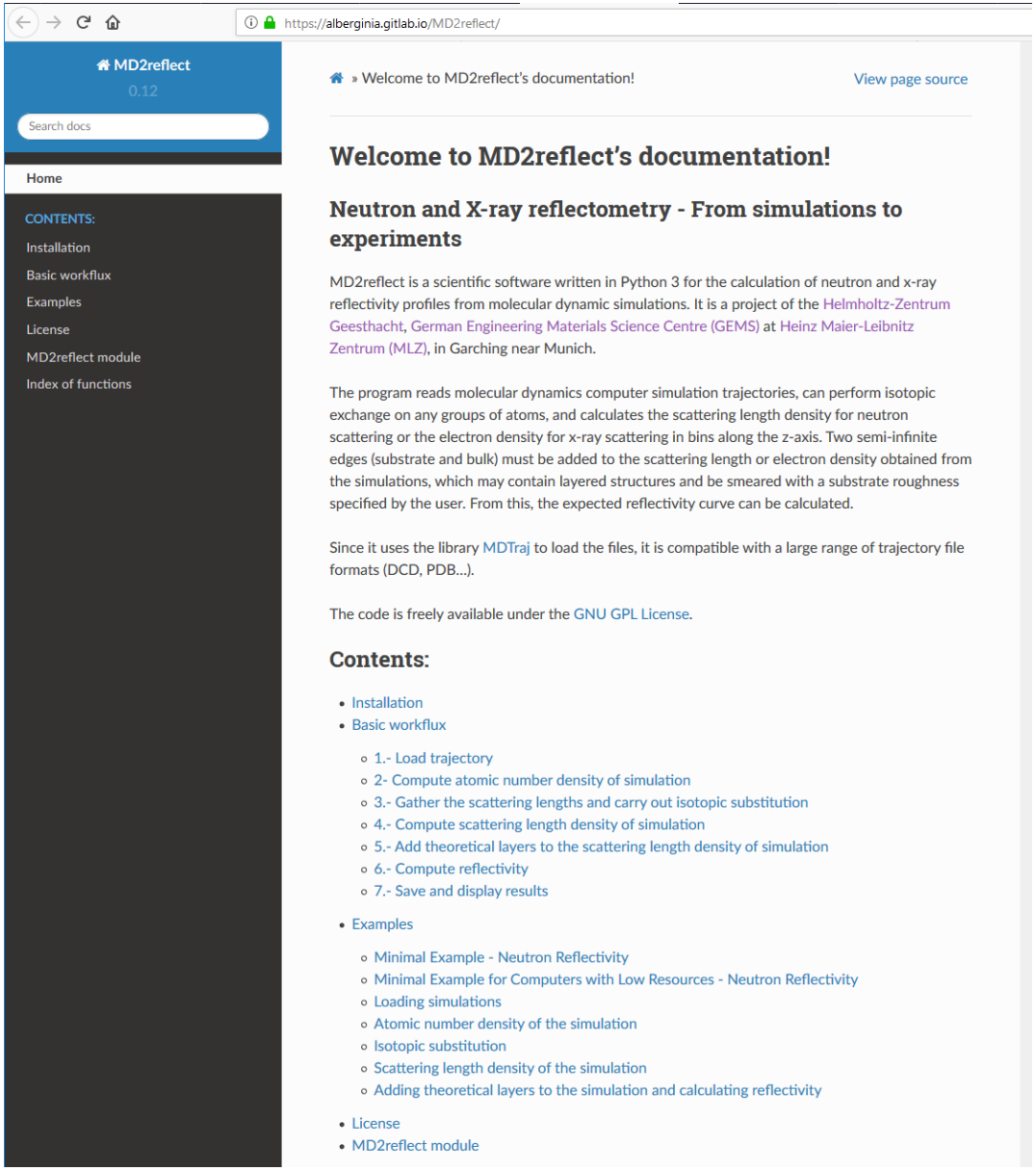




Average over 12 replicas with a different starting configuration






https://alberginia.gitlab.io/MD2reflect/
MD2reflect
0.12
Search docs
Home
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Installation
Basic workflux
Examples
License
MD2reflect module
Index of functions
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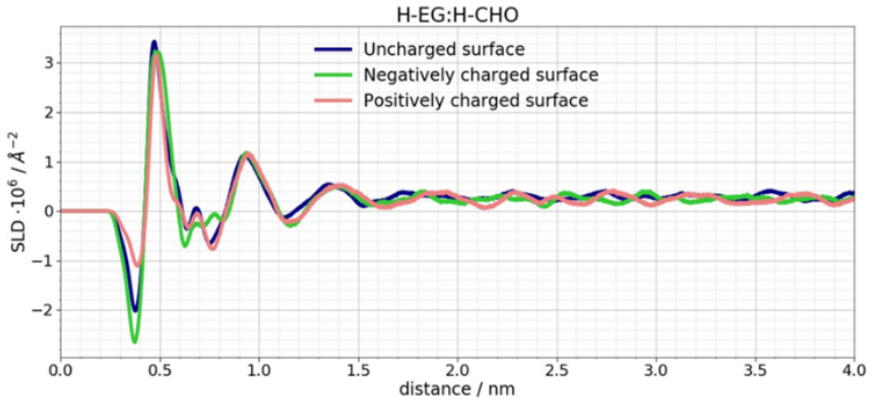
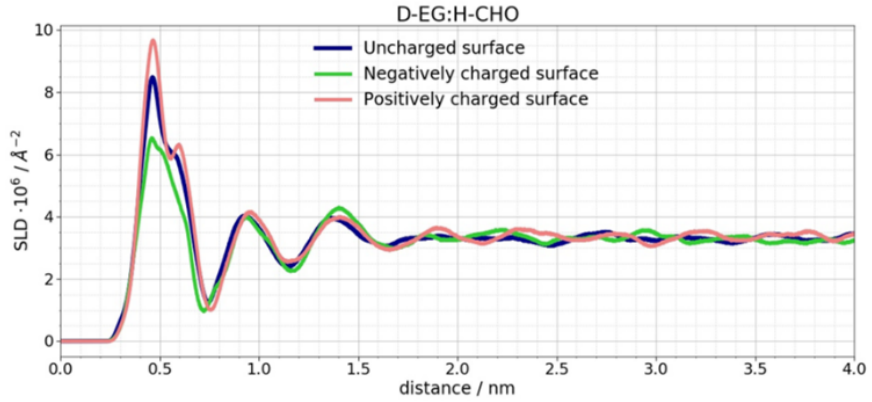
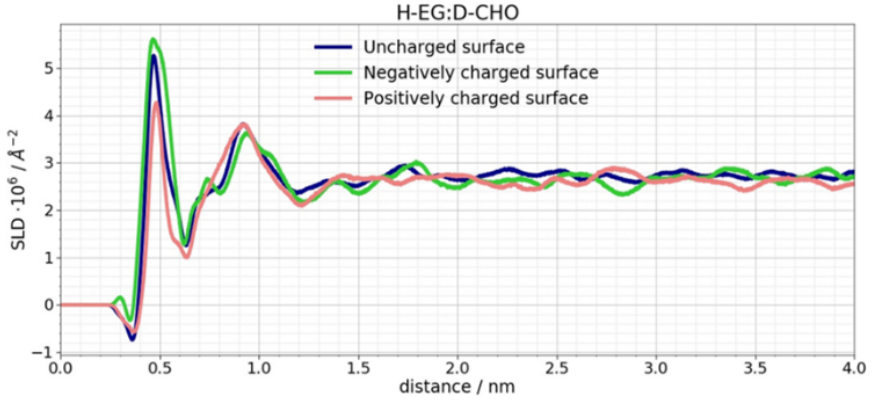
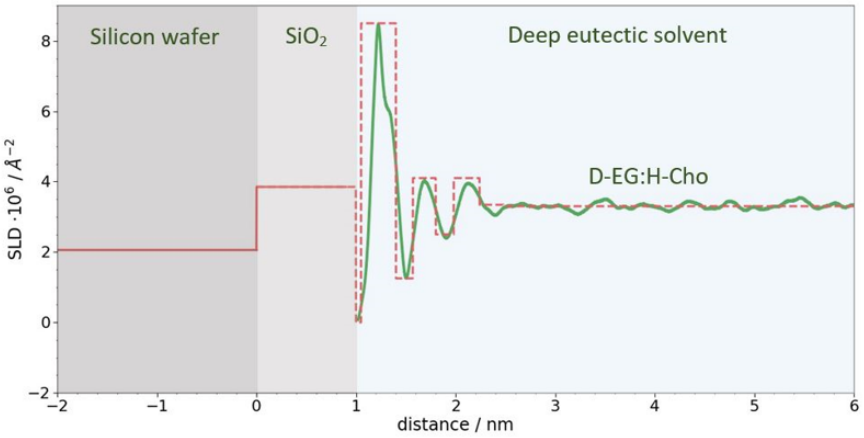
Neutron and X-ray reflectometry - From simulations to experiments
MD2reflect is a scientific software written in Python 3 for the calculation of neutron and x-ray reflectivity profiles from molecular dynamic simulations. It is a project of the Helmholtz-Zentrum Geesthacht, German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), in Garching near Munich.
The program reads molecular dynamics computer simulation trajectories, can perform isotopic exchange on any groups of atoms, and calculates the scattering length density for neutron scattering or the electron density for x-ray scattering in bins along the z-axis. Two semi-infinite edges (substrate and bulk) must be added to the scattering length or electron density obtained from the simulations, which may contain layered structures and be smeared with a substrate roughness specified by the user. From this, the expected reflectivity curve can be calculated.
Since it uses the library MDTraj to load the files, it is compatible with a large range of trajectory file formats (DCD, PDB...).
The code is freely available under the GNU GPL License.
Contents:
Installation
Basic workflux
1.- Load trajectory
2- Compute atomic number density of simulation
3.- Gather the scattering lengths and carry out isotopic substitution
4.- Compute scattering length density of simulation
5.- Add theoretical layers to the scattering length density of simulation
6.- Compute reflectivity
7.- Save and display results
Examples
Minimal Example - Neutron Reflectivity
Minimal Example for Computers with Low Resources - Neutron Reflectivity
Loading simulations
Atomic number density of the simulation
Isotopic substitution
Scattering length density of the simulation
Adding theoretical layers to the simulation and calculating reflectivity
License
MD2reflect module

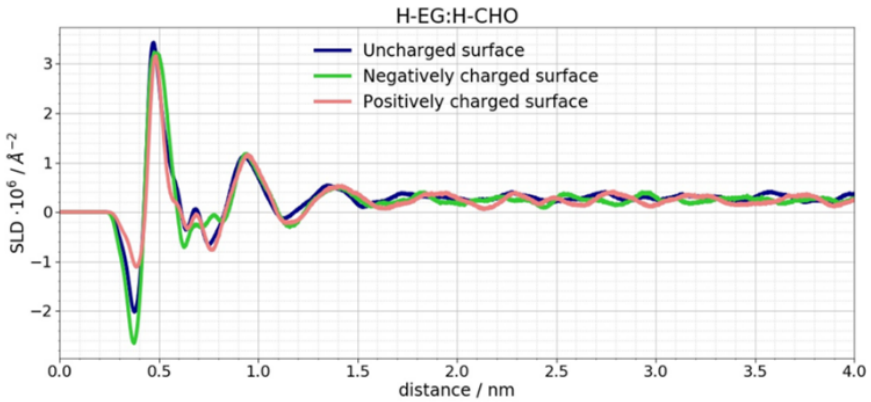

H-EG:H-CHO
Uncharged surface
Negatively charged surface
Positively charged surface
SLD ·10⁶ / Å⁻²
distance / nm

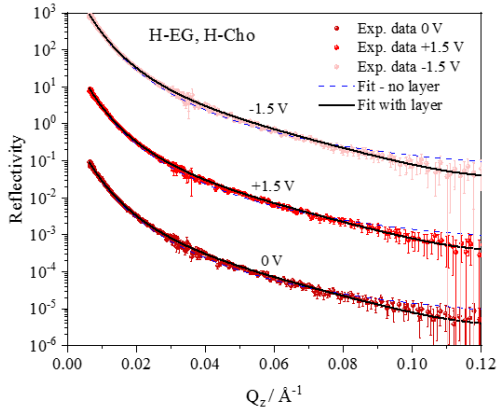

D-EG:H-CHO
Uncharged surface
Negatively charged surface
Positively charged surface
SLD ·10⁶ / Å⁻²
distance / nm

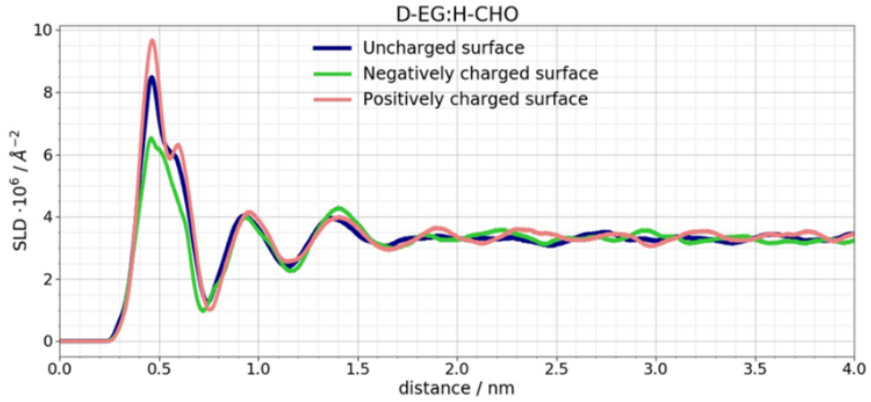

H-EG:D-CHO
Uncharged surface
Negatively charged surface
Positively charged surface
SLD ·10⁶ / Å⁻²
distance / nm

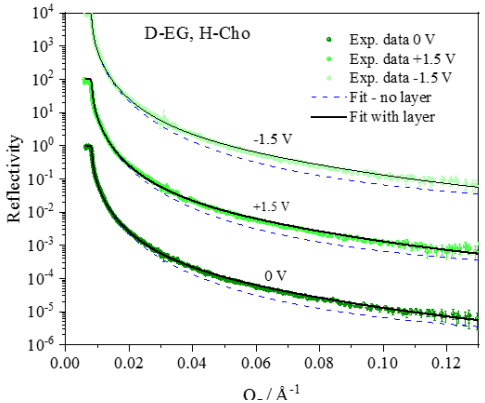
“crude model”

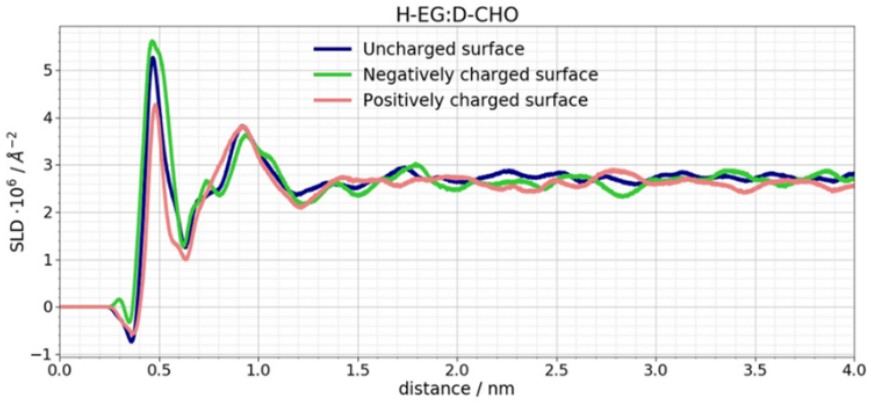

Silicon wafer
SiO2
Deep eutectic solvent
D-EG:H-Cho
SLD ·10⁶ / Å⁻²
distance / nm

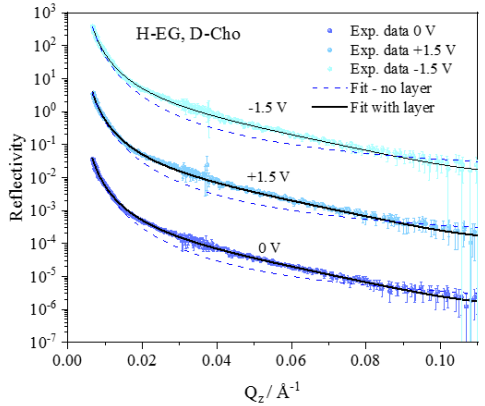

H-EG:H-CHO
Uncharged surface
Negatively charged surface
Positively charged surface
SLD ·10⁶ / Å⁻²
distance / nm

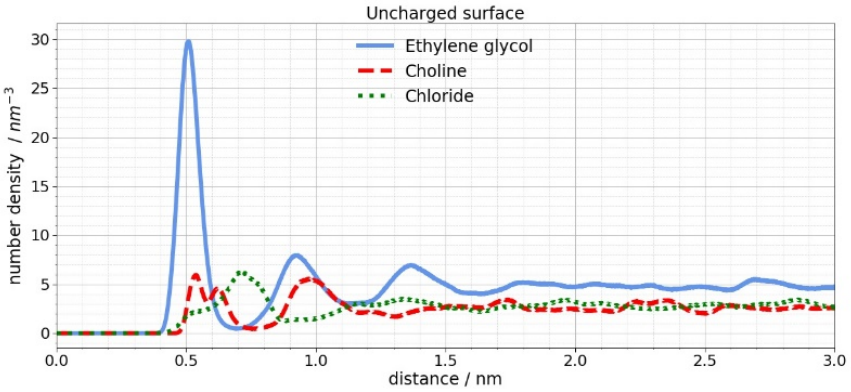

H-EG, H-Cho
Exp. data 0 V
Exp. data +1.5 V
Exp. data -1.5 V
Fit - no layer
Fit with layer
-1.5 V
+1.5 V
0 V
Reflectivity
Q_z / Å⁻¹

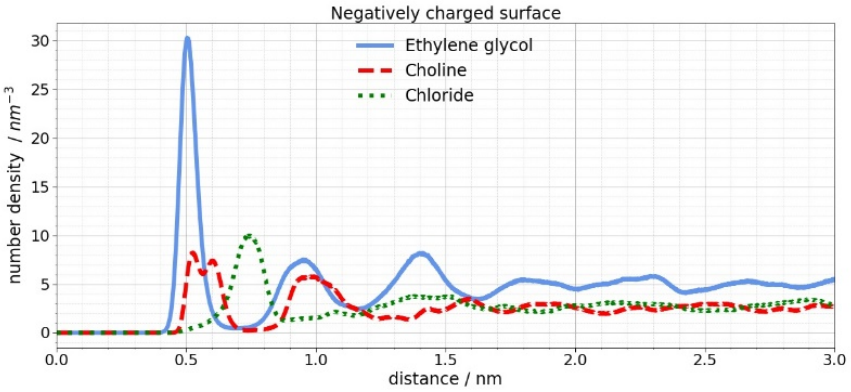

D-EG:H-CHO
Uncharged surface
Negatively charged surface
Positively charged surface
SLD ·10⁶ / Å⁻²
distance / nm

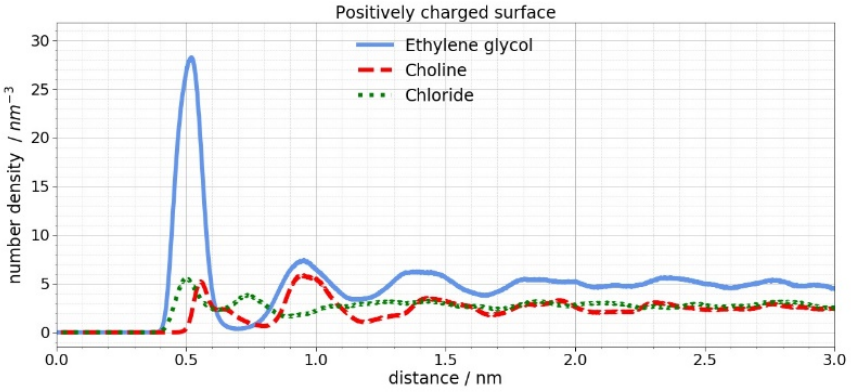

D-EG, H-Cho
Exp. data 0 V
Exp. data +1.5 V
Exp. data -1.5 V
Fit - no layer
Fit with layer
-1.5 V
+1.5 V
0 V
Reflectivity
Q_z / Å⁻¹


H-EG:D-CHO
Uncharged surface
Negatively charged surface
Positively charged surface
SLD ·10⁶ / Å⁻²
distance / nm

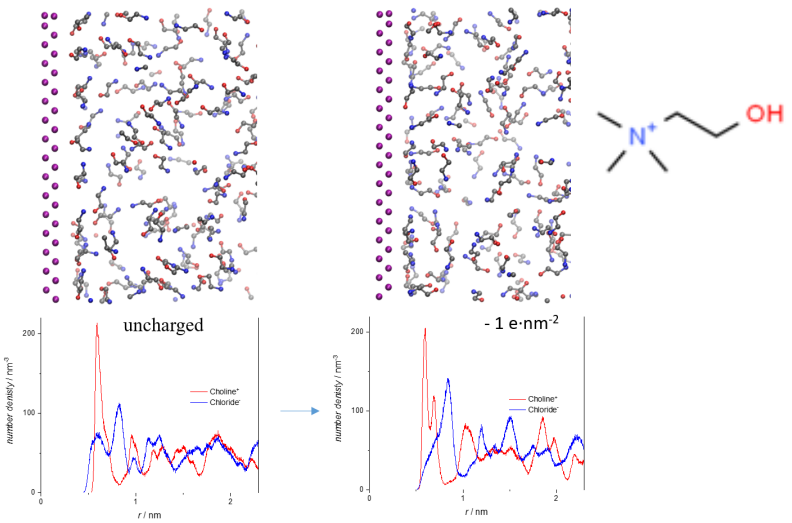

H-EG, D-Cho
Exp. data 0 V
Exp. data +1.5 V
Exp. data -1.5 V
Fit - no layer
Fit with layer
-1.5 V
+1.5 V
0 V
Reflectivity
Q_z / Å⁻¹



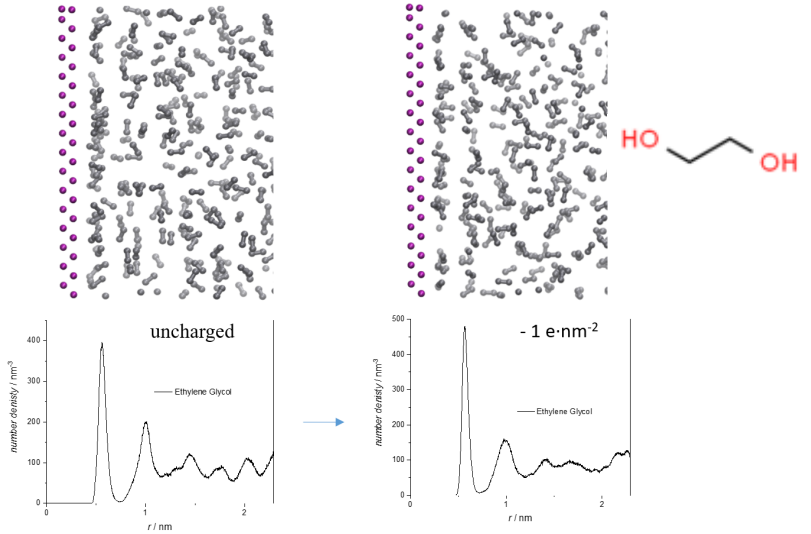




Choline – N-C-C-O



Ethylene glycol – C-C



Thank you for your attention!

Questions?