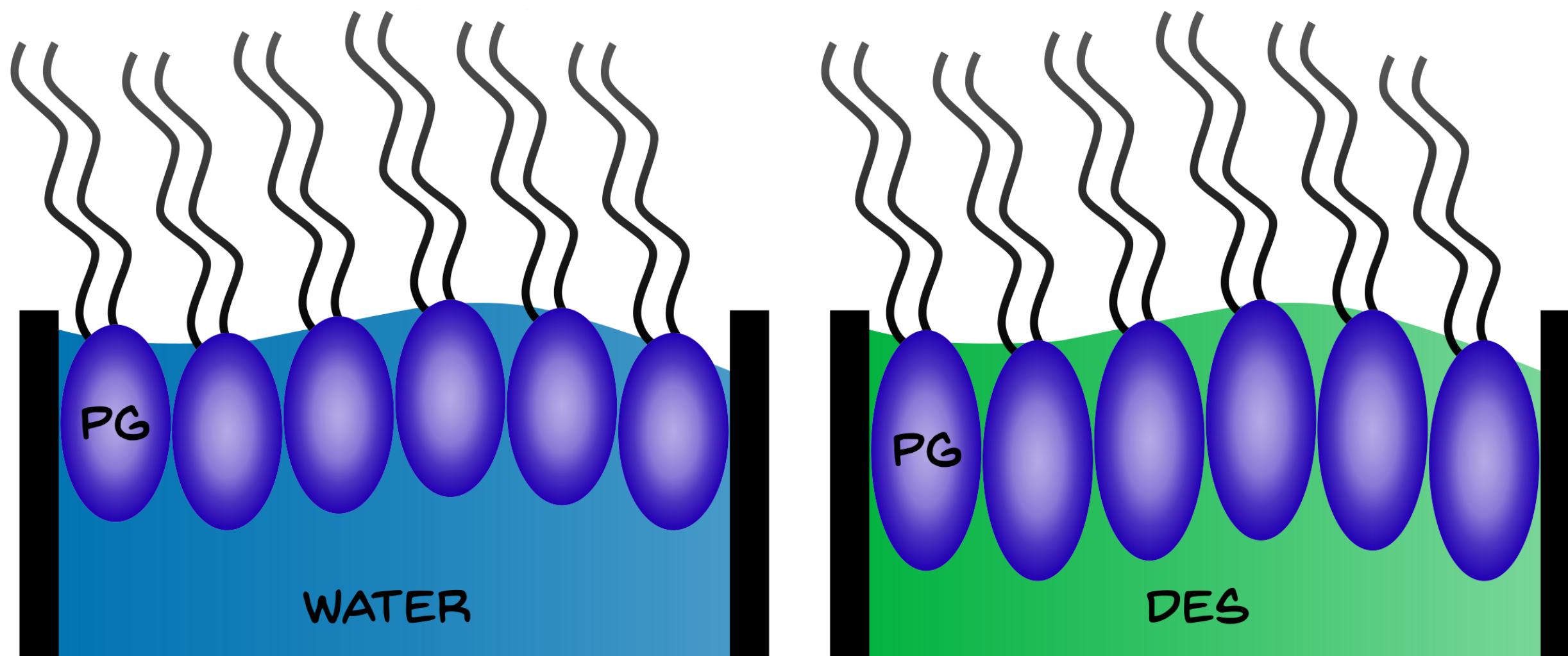


ANDREW R. MCCLUSKEY

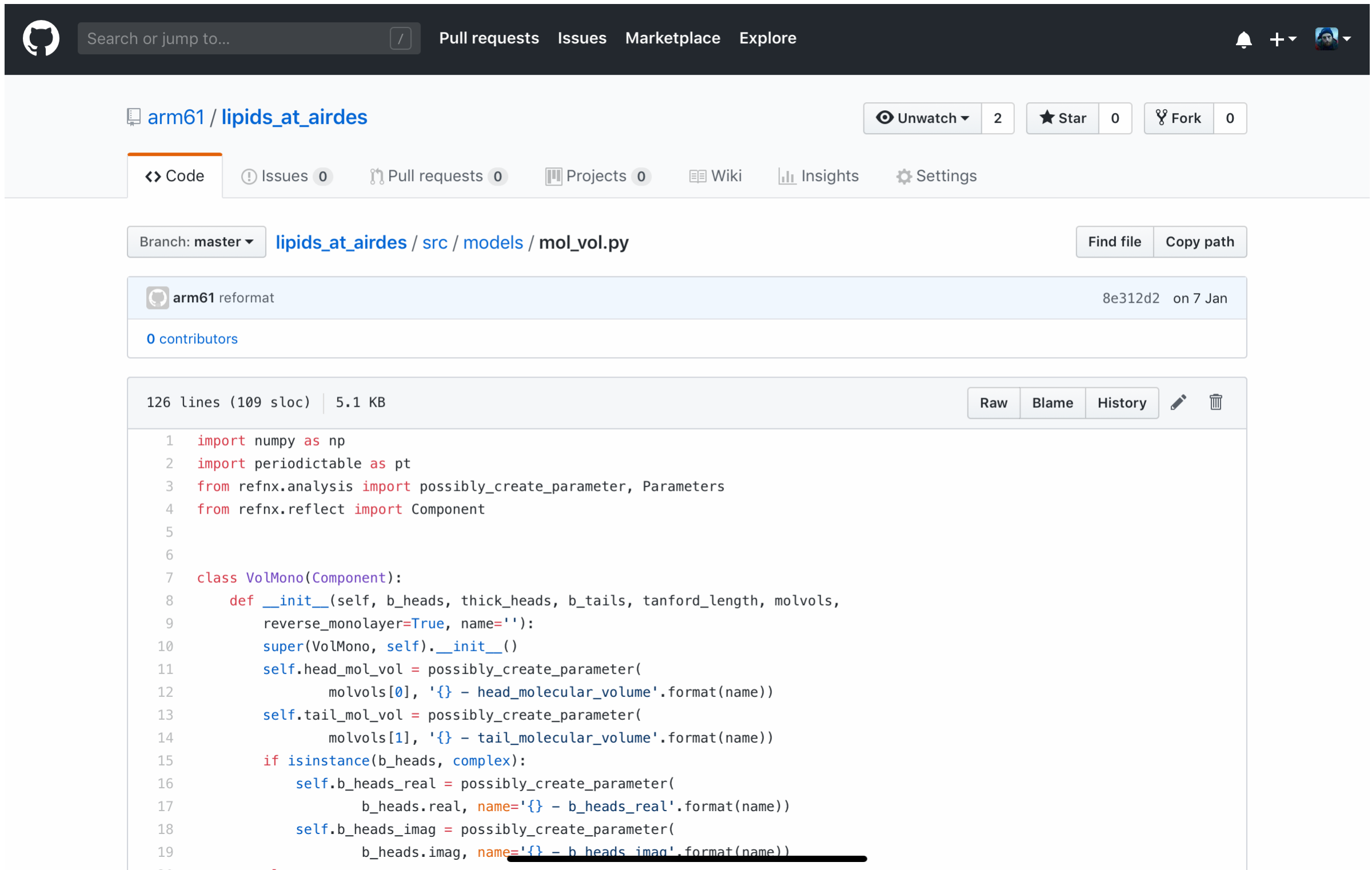
DIAMOND LIGHT SOURCE & UNIVERSITY OF BATH

BAYES FOR REFLECTOMETRY AND OTHER THOUGHTS

LIPID MONOLAYERS



Phys. Chem. Chem. Phys., 2019, **21**(11) 6133-6141. DOI: 10.1039/C9CP00203K



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arm61 / lipids_at_airdes

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Branch: master lipids_at_airdes / src / models / mol_vol.py Find file Copy path

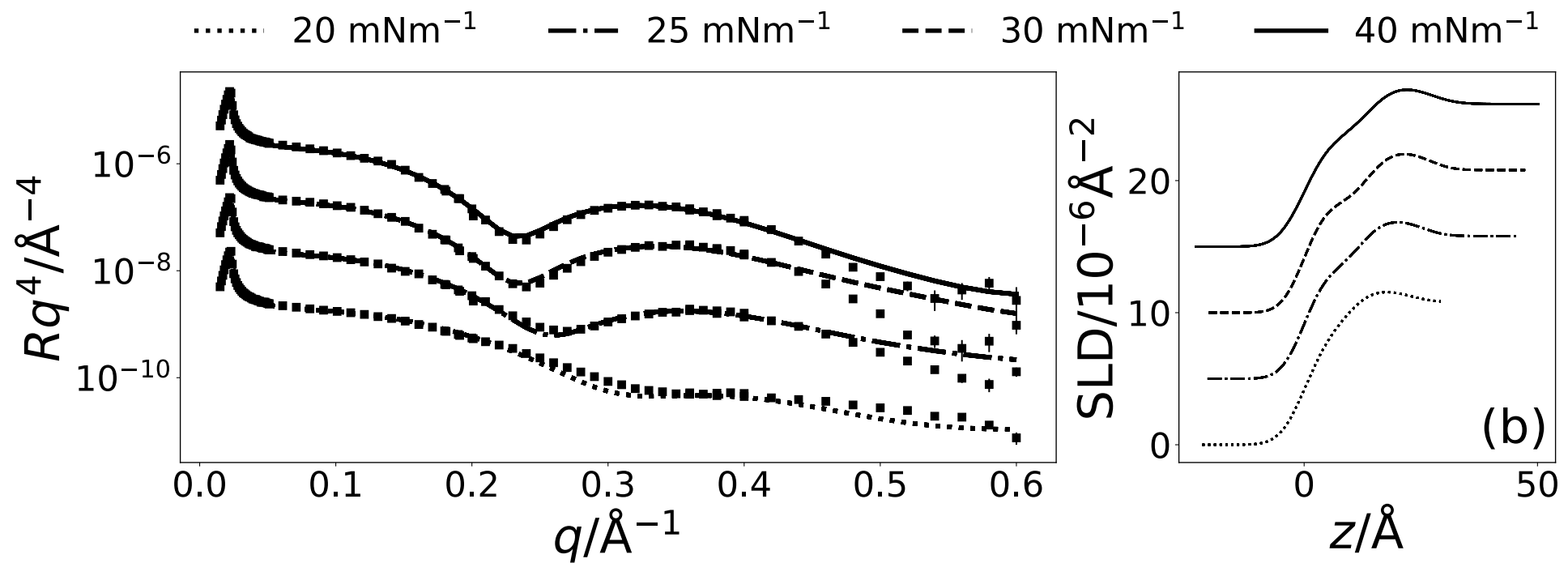
arm61 reformat 8e312d2 on 7 Jan

0 contributors

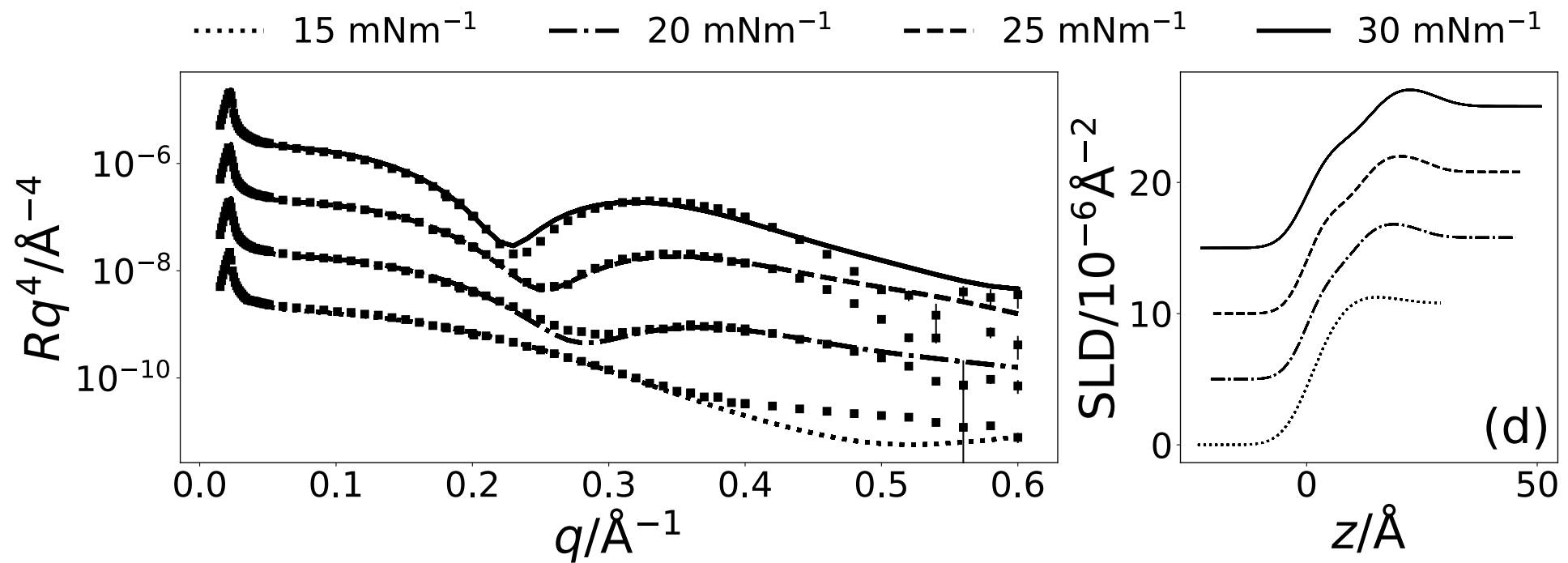
126 lines (109 sloc) | 5.1 KB Raw Blame History

```
1 import numpy as np
2 import periodictable as pt
3 from refnx.analysis import possibly_create_parameter, Parameters
4 from refnx.reflect import Component
5
6
7 class VolMono(Component):
8     def __init__(self, b_heads, thick_heads, b_tails, tanford_length, molvols,
9                 reverse_monolayer=True, name=''):
10        super(VolMono, self).__init__()
11        self.head_mol_vol = possibly_create_parameter(
12            molvols[0], '{} - head_molecular_volume'.format(name))
13        self.tail_mol_vol = possibly_create_parameter(
14            molvols[1], '{} - tail_molecular_volume'.format(name))
15        if isinstance(b_heads, complex):
16            self.b_heads_real = possibly_create_parameter(
17                b_heads.real, name='{} - b_heads_real'.format(name))
18            self.b_heads_imag = possibly_create_parameter(
19                b_heads.imag, name='{} - b_heads_imag'.format(name))
20        ..
```

github.com/arm61/lipids_at_airdes



Lipid = DMPC

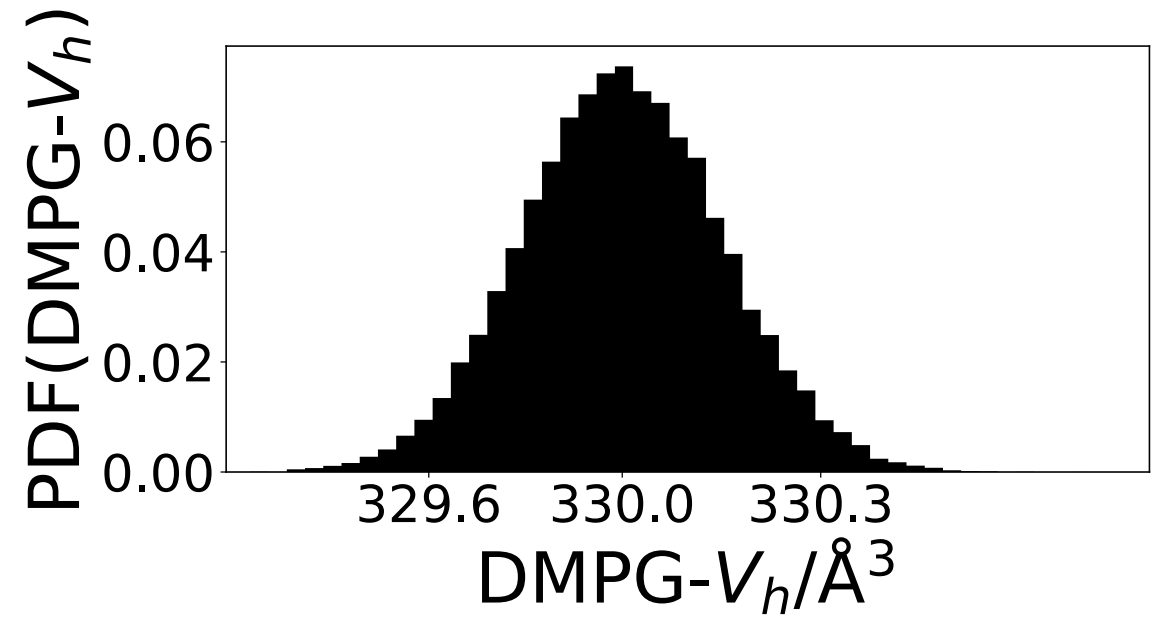
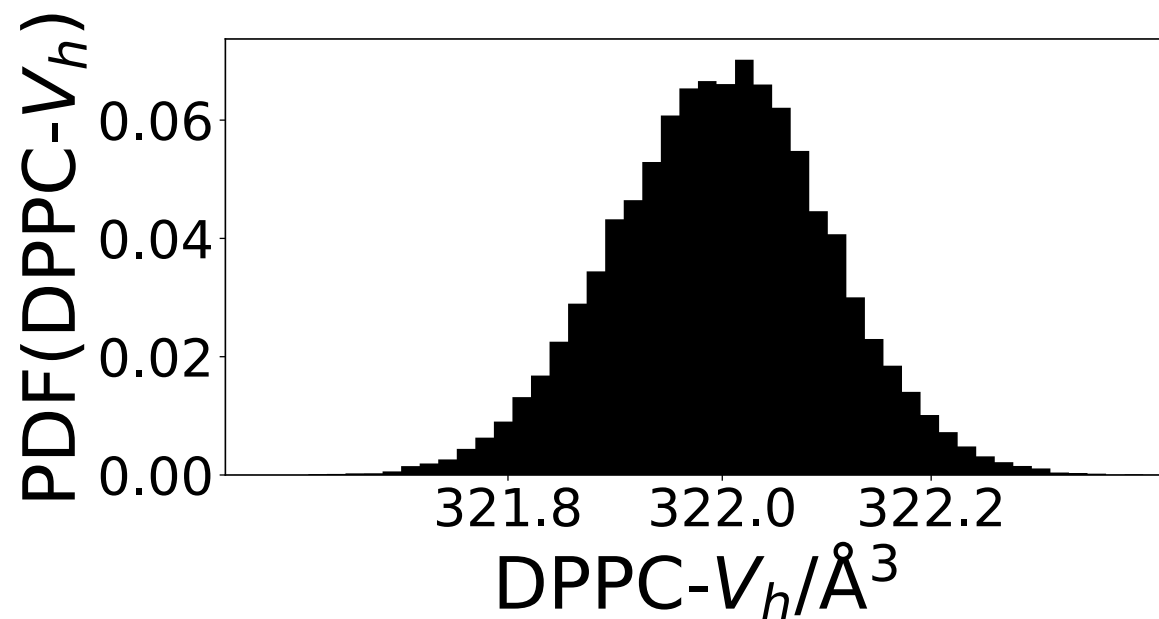
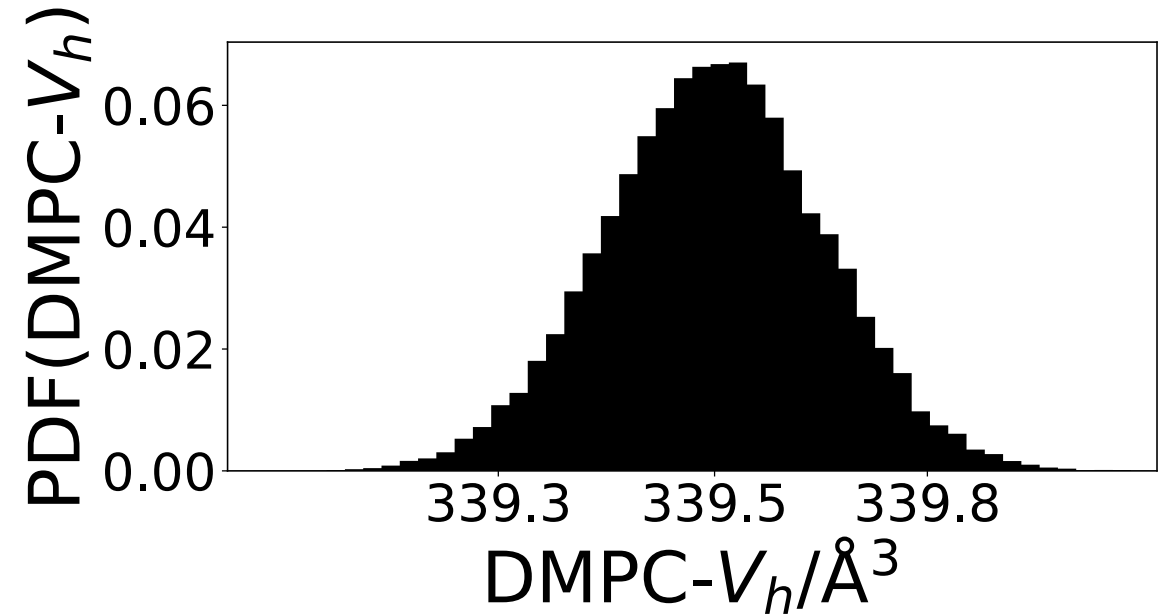
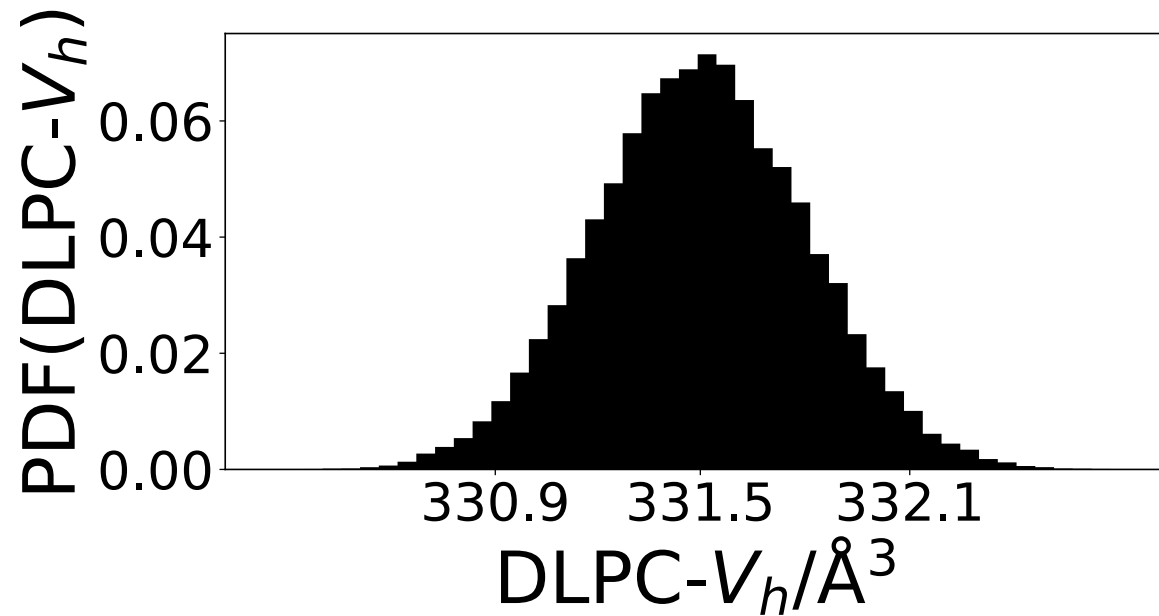


Lipid = DMPG



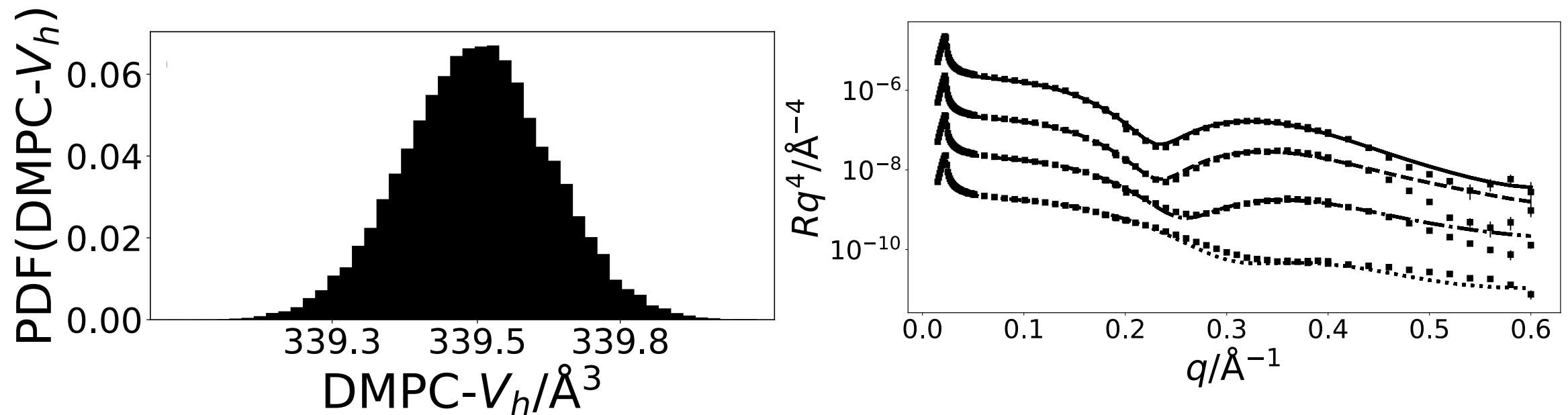
Goodman & Weare's Affine Invariant Markov
chain Monte Carlo Ensemble sampler for
Bayesian parameter estimation

BAYESIAN PARAMETER ESTIMATION



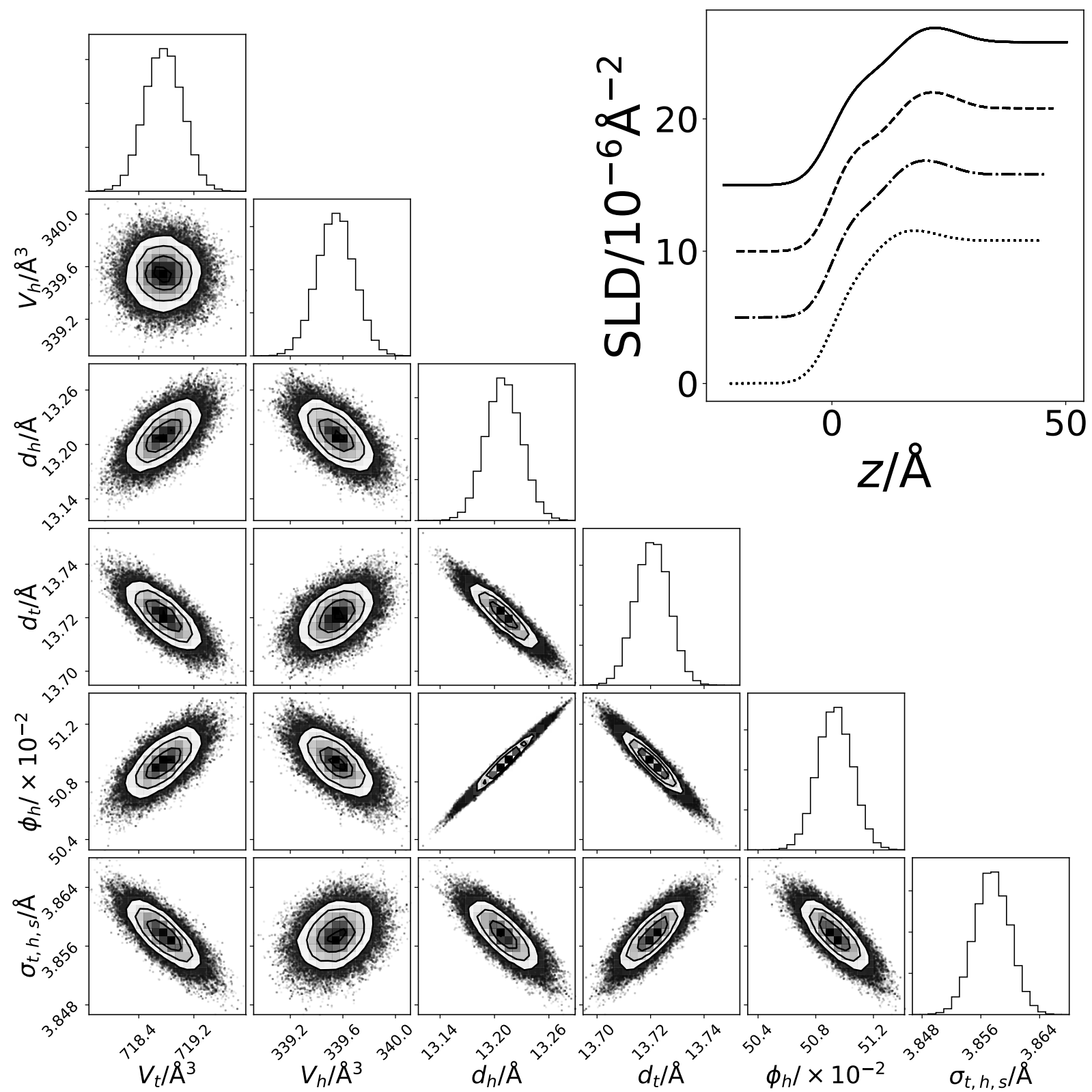
Previously the V_h for DMPG was shown to be 291 \AA^3

BAYESIAN PARAMETER ESTIMATION



Parameter variance is substantially underestimated due to uncertainty underestimation in the experimental data

We need to better understand the uncertainty in the experimental measurement



CONCLUSIONS

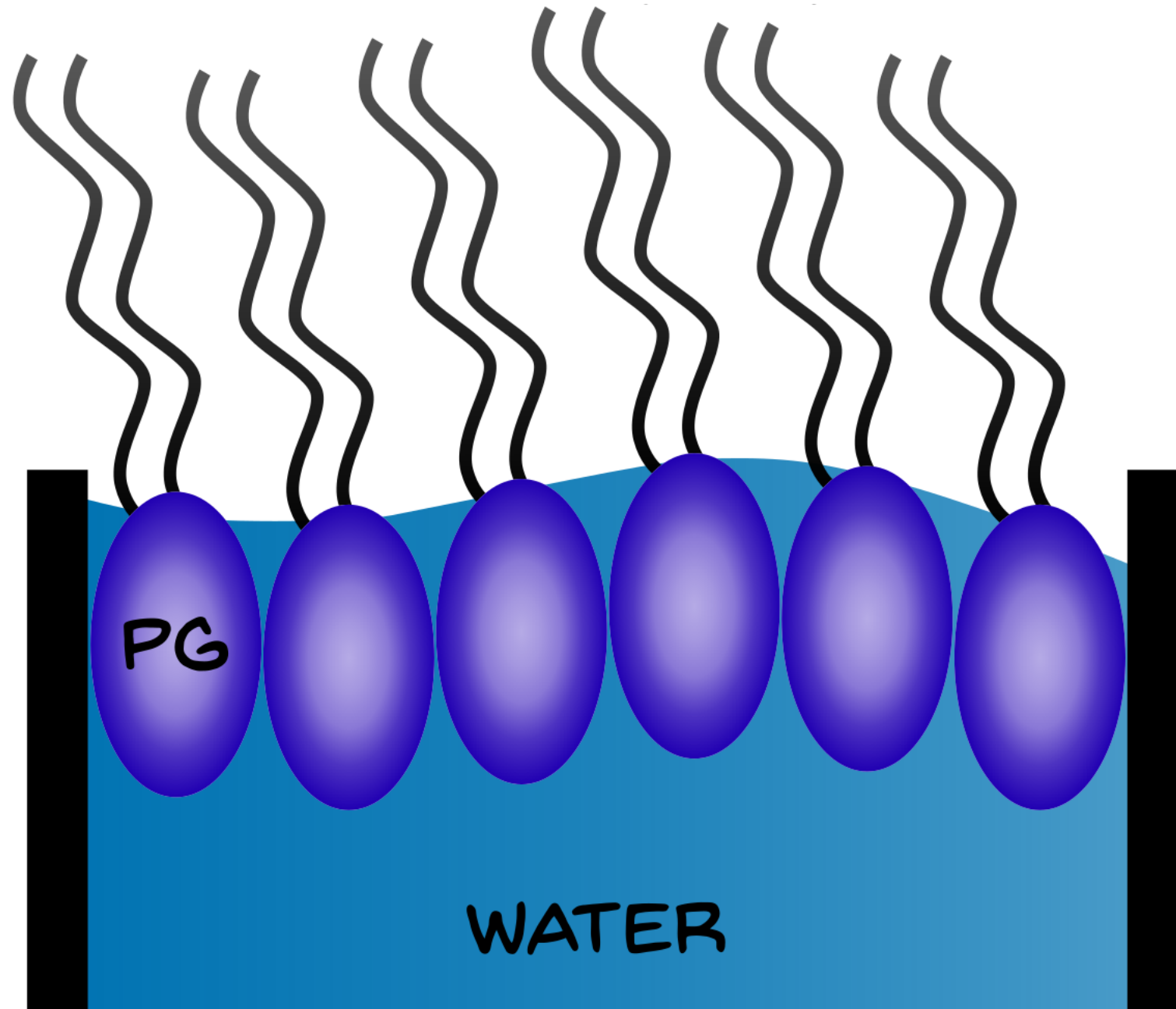
- ▶ A chemically-consistent reflectometry model was used to investigate the structure of a lipid monolayer at a non-aqueous interface
- ▶ Model optimisation was achieved with co-refinement of multiple datasets and differential evolution algorithm
- ▶ Markov chain Monte Carlo was used for Bayesian parameter estimation with limited success due to underestimation of experimental uncertainties
- ▶ Bayesian parameter estimation did allow for a better understanding of parametric correlations

Paper: ***Phys. Chem. Chem. Phys.***, 2019, **21**(11) 6133-6141.

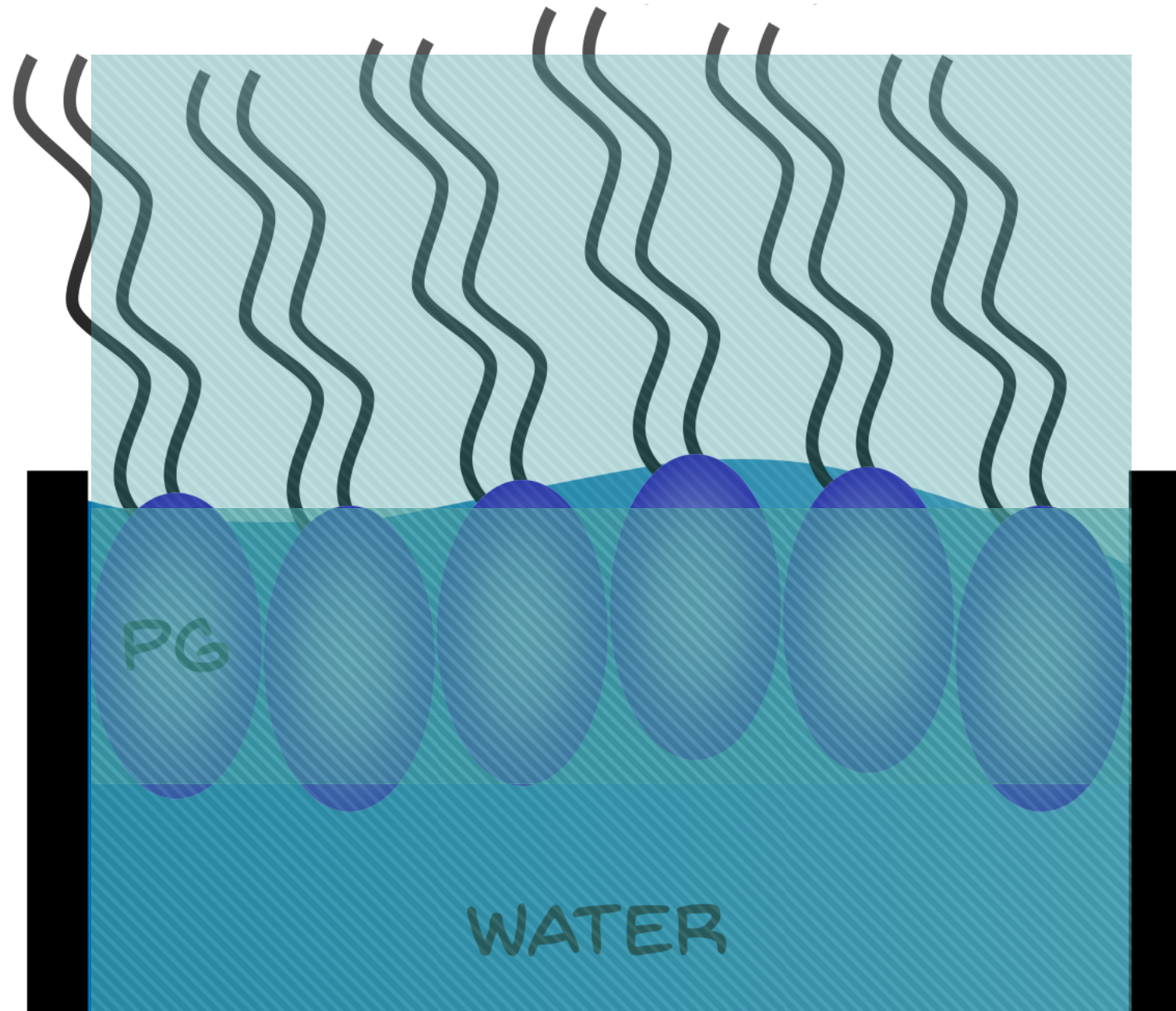
DOI: 10.1039/C9CP00203K

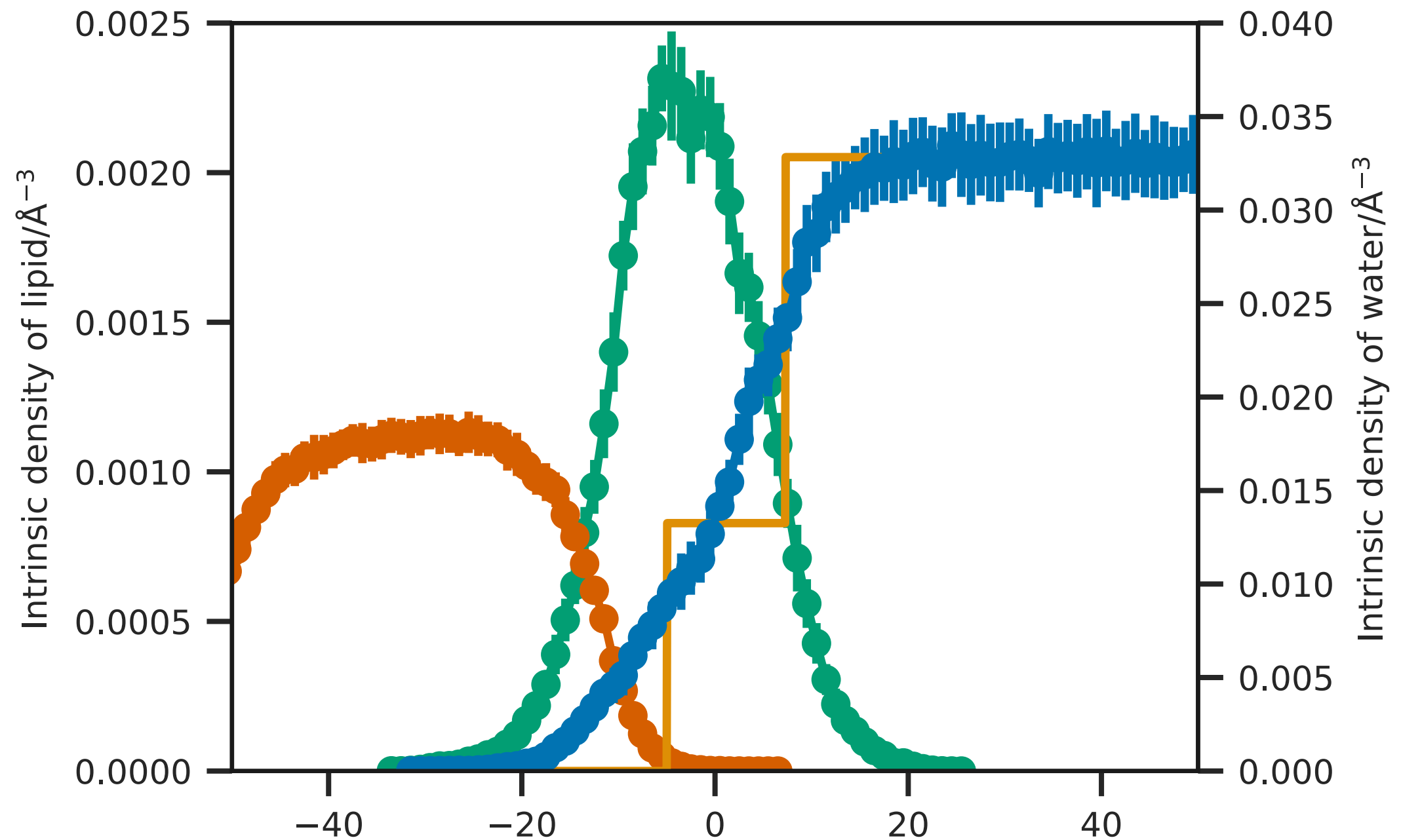
GitHub: github.com/arm61/lipids_at_airdes

OTHER BAYESIAN APPLICATIONS

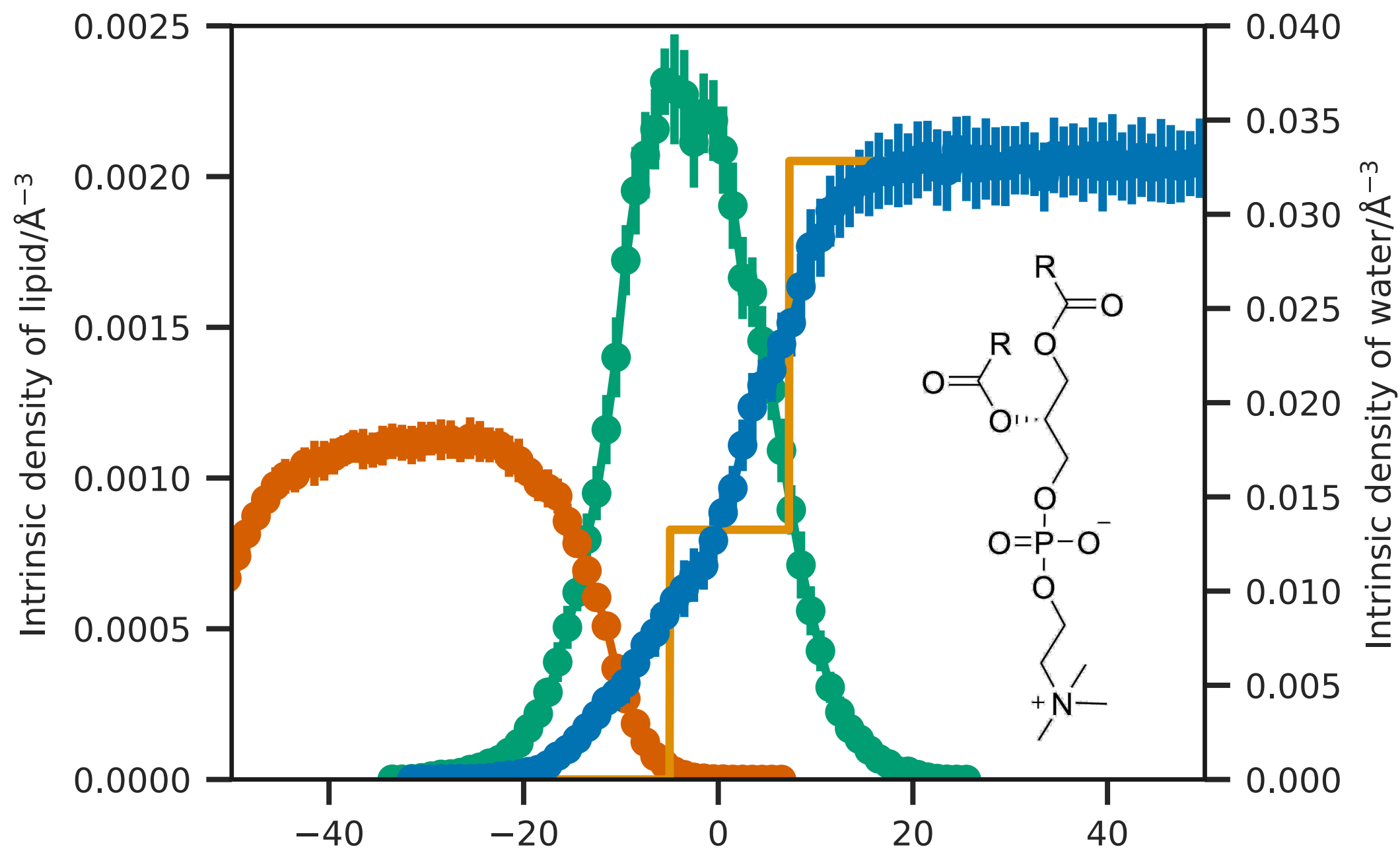


LIPID MONOLAYER MODELS





J. Phys. Comm., 2019, Accepted. DOI: 10.1088/2399-6528/ab12a9



J. Phys. Comm., 2019, Accepted. DOI: 10.1088/2399-6528/ab12a9

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- ▶ Organisers and yourselves



Sadie and Penny