Computational Screening of Soft Materials Systems with Application to Nano-Lubrication Systems

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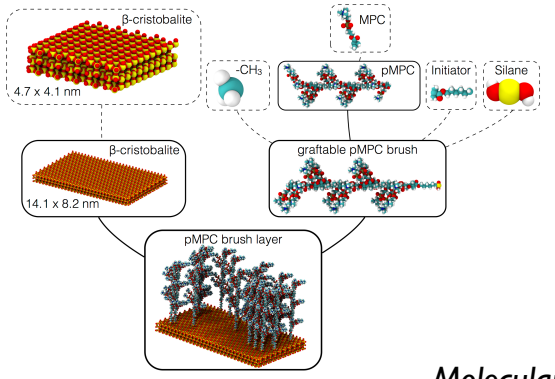
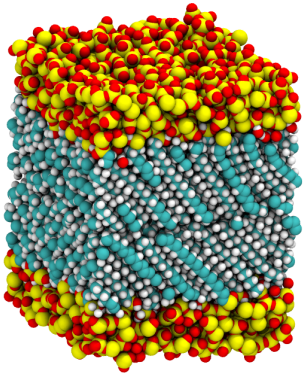




SCHOOL OF ENGINEERING

Telluride Science Research Center Workshop

Molecular engineering of soft matter: Spanning small molecules to macromolecules

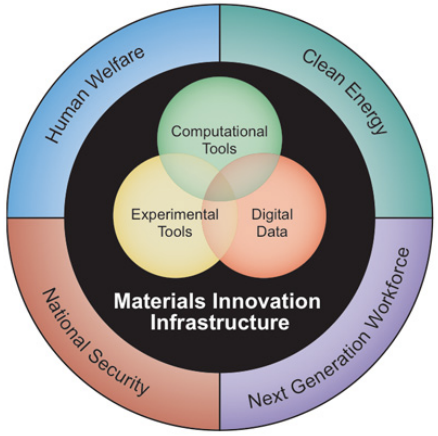
Telluride, CO

June 19-24, 2017

MUMS

Motivation - Computational Materials Discovery

- Computational discovery of new materials is emerging as new subfield of computational materials science developing out of the Materials Genome Initiative (MGI), e.g.:
  - **The Materials Project**
    - https://materialsproject.org
    - Properties of over 80,000 materials and screened 25,000 of these for Li-ion batteries.
      - *Based on use of low-level electronic structure methods on crystalline (ordered) materials*
  - **Screening of metal-organic frameworks (MOFs)[1]**
    - 137,953 hypothetical MOF structures generated
      - *Each MOF evaluated for methane storage at 35 bar and 298 K using grand canonical Monte Carlo*
    - ~300 MOFs had higher methane-storage capacity at 35 bar than current world record
  - **Crowdsourced Clean Energy Project database at H**
    - http://www.molecularspace.org
    - Data and analyses on 2.3 million candidate compounds for organic photovoltaics
      - *Ab initio methods applied to single molecules, linking structural and electronic properties*



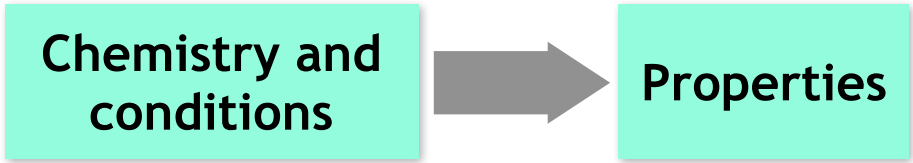
https://www.mgi.gov/sites/default/files/documents/materials_genome_initiative-final.pdf

Chemistry and conditions → **Properties**

[1] Wilmer, et al., Large-scale screening of hypothetical metal–organic frameworks. Nature Chemistry, 4 (2011) 83-89. doi:10.1038/nchem.1192

Motivation - MGI for Soft Matter

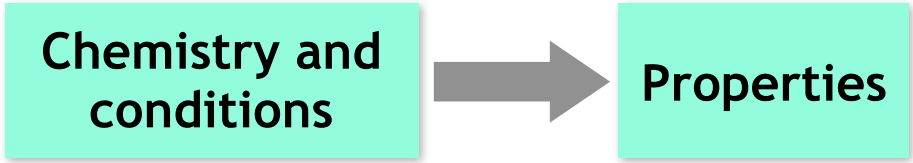
- In soft matter, predominant physical behaviors occur at energy scales comparable with k_BT
  Quantum aspects generally unimportant
  - Weak dispersion interactions frequently dominate
    - Contrast with hard materials
      - *Energy scales large by comparison to k_BT*
      - *Relatively easy to predict properties since atoms/molecules are typically in crystalline lattice*
  - It can be difficult to predict properties directly from atomic or molecular constituents
    - Soft matter often self-organizes into mesoscopic physical structures that are much larger than microscopic scale yet much smaller than the macroscopic scale
      - *Macroscopic properties are result of mesoscopic structure*
      - *Hard materials typically have no mesoscopic structuring*
    - Many steps are needed to gather properties based on a given chemistry and condition



MoSDeF

The Molecular Simulation and Design Framework

- Motivation - develop a platform for performing MGI-style screening of soft-matter systems
  - Goal:

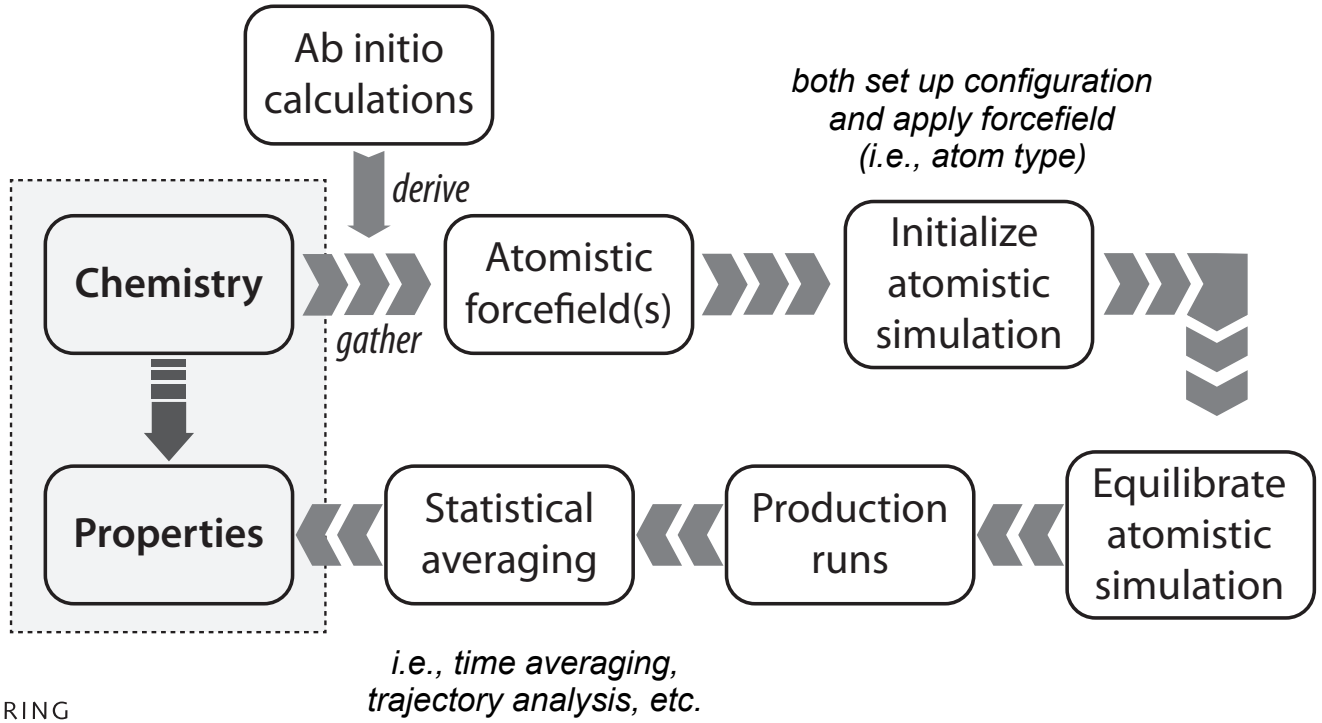


  - The procedures grouped into the arrow can be considered a "cottage industry" that is not always easy to reproduce
    - Only a few people have the knowledge to reproduce the specific simulation
      - *Procedures are not always well documented/described*
      - *The properties may depend on the exact details of the procedures*
    - *Ad hoc* tools/scripts are not always made available
      - *Software may be highly specific and not extensible*
      - *Software may be poorly written and not be well validated*

MoSDeF

A Molecular Simulation and Design Framework

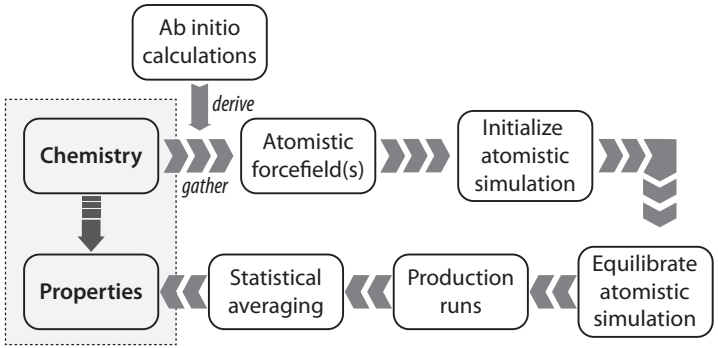
- **Motivation** - develop a platform for performing Materials Genome Initiative (MGI) style screening of soft-matter systems



MoSDeF

A Molecular Simulation and Design Framework

- **Motivation** - develop a platform for performing Materials Genome Initiative (MGI) style screening of soft-matter systems
  - To do so, need to automate each of these steps and be able to combine them together
    - Model-Integrated Computing (MIC)
    - Developed by Vanderbilt researchers in the Institute for Software Integrated Systems (ISIS)
    - Used in wide variety of applications where scientific/engineering workflows require automation and integration to achieve complex goals
      - *Car manufacturing assembly line automation and control (GM)*
      - *Health records management (NIH)*
      - *Amphibious infantry fighting vehicle design (DARPA)*
    - MIC involves meta-language abstraction
  - MoSDeF is outgrowth of three NSF grants joint with ISIS
    - NSF CDI CBET 1028374, NSF SSI ACI 1047828, NSF SSE ACI 1535150
    - MoSDeF also seeks to address **simulation reproducibility**



Sztipanovits, J. Karsai, G., "Model-integrated computing," *Computer*, **30**, 110-111 (1997)

MoSDeF

A Molecular Simulation and Design Framework

- Why does MoSDeF promote simulation reproducibility and why is this important?
  - In a science-skeptic world, the "reproducibility crisis" in scientific research has emerged as critical issue
    - http://www.nature.com/news/reproducibility-1.17552
  - Reproducibility in computational science is becoming a forefront issue in the computational science community
    - Automation is a key device for reproducibility
      - *Sandve, G. K. et al. (2013), Ten simple rules for reproducible computational research, PLOS Comp. Bio. (editorial), Vol. 9(10):1–4, doi: 10.13711/journal.pcbi.1003285*
    - "Reproducible computational research, in which all details of computations—code and data—are made conveniently available to others, is a necessary response to [the credibility] crisis."
      - *Donoho, D. et al. (2009), Reproducible research in computational harmonic analysis, Comp. Sci. Eng. 11(1):8–18, doi: 10.1109/MCSE.2009.15*
    - GUIs are the enemy of reproducibility
      - *Lorena A. Barba, George Washington University; see her blog http://lorenabarba.com/category/blog/ and "The hard road to reproducibility", Science, 354(6308):142 (October 2016)*
  - Scriptability, open-source, complete data dissemination needed to reproduce published simulations are goals inherent to MoSDeF

MoSDeF

A Molecular Simulation and Design Framework

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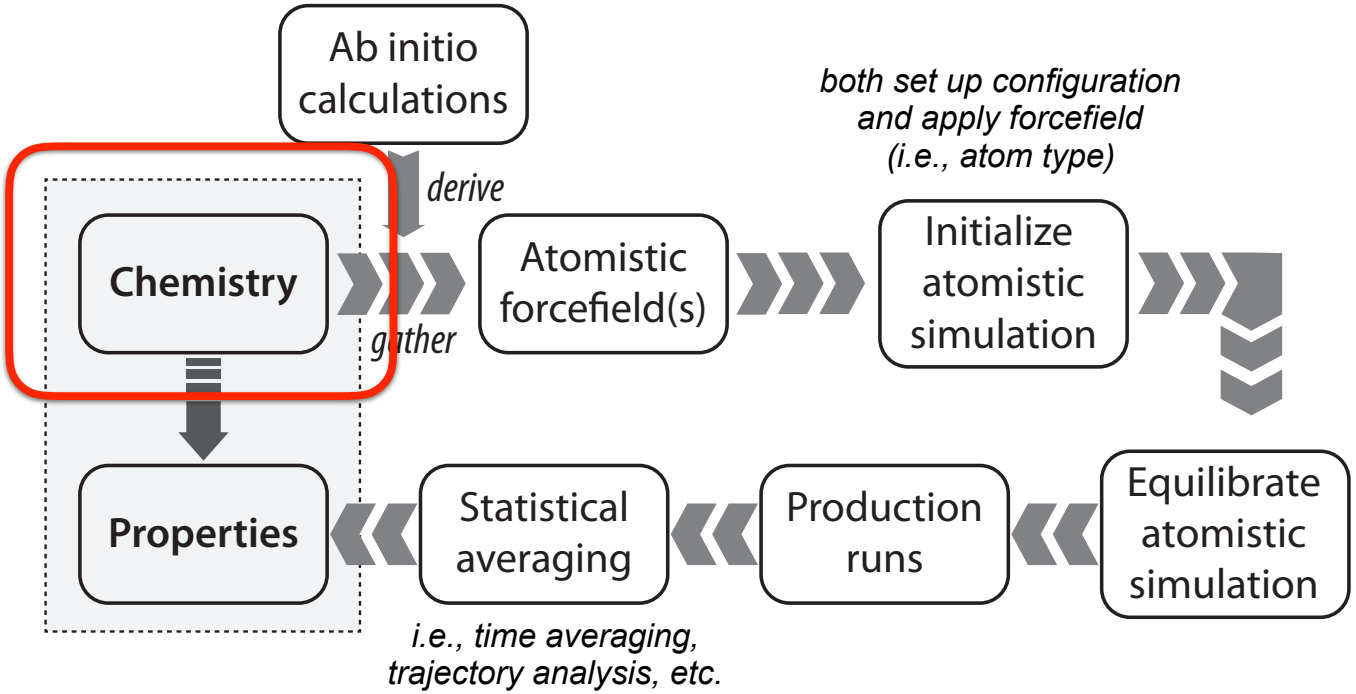
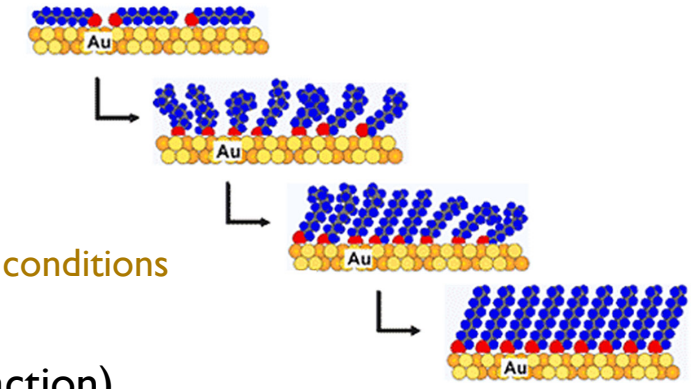


Missing Functionality in Existing Tools

- Surface functionalization
  - Need ability to express patterns
  - Expose parameters that tune chemistry
- Flexible force field development and dissemination
  - Few force fields exist for all chemistries we care about
  - Not certain how accurate existing FFs will behave under high shear conditions
  - Collaborators and group members developing for specific systems
- Desire to use different simulation engines (meta-level abstraction)
  - LAMMPS, HOOMD, Gromacs all currently used in group
- MoSDeF is open source, built on open source components

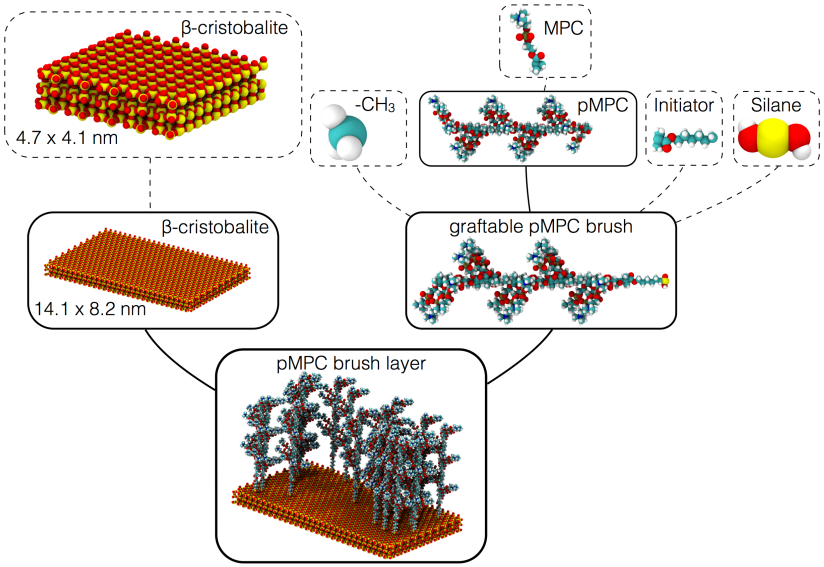


Nuzzo *et al.*, *JACS*, **1983**, *105*

NumPy SciPy matplotlib IPython Interactive Computing pandas scikit learn

mBuild: a Hierarchical Molecular Builder

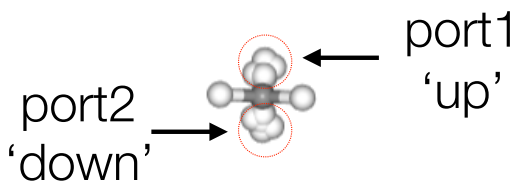
- Sketch or otherwise create simple components (dashed boxes)
- Combine operations on components into more complicated structures
  - Our applications (nanotribology, supercapacitors, skin lipid self-assembly) typically involve interfacial systems
- Everything is scriptable



https://github.com/mosdef-hub/mbuild.git

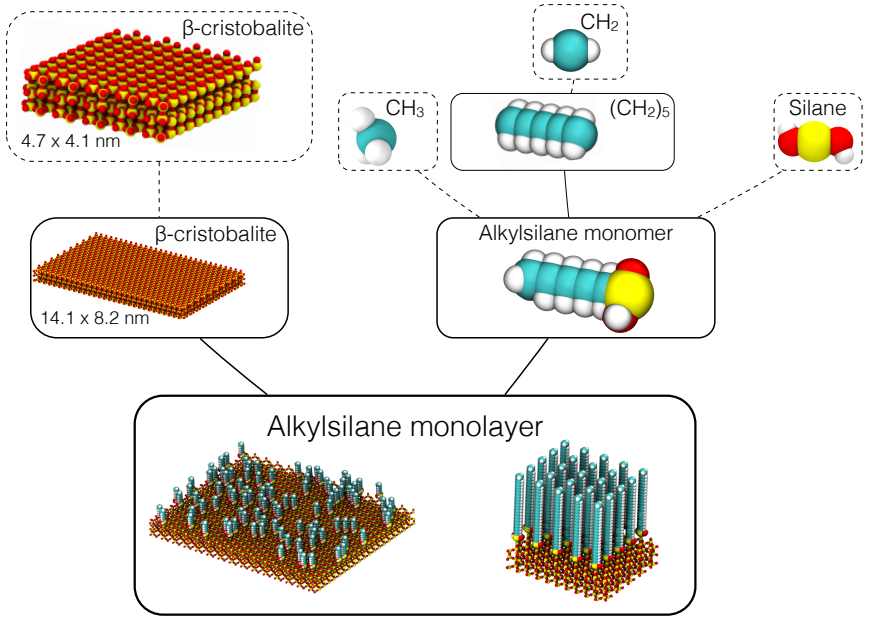
Example: polymerization

```
import mbuild as mb
from mbuild.lib.moieties import CH2

polymer = mb.Compound()

last_monomer = CH2()
polymer.add(last_monomer)

for _ in range(10):
    current_monomer = mb.clone(last_monomer)

    mb.force_overlap(move_this=current_monomer,
                     from_port=current_monomer['up'],
                     to_port=last_monomer['down'])

    polymer.add(current_monomer)
    last_monomer = current_monomer
```



- Above code with additional features is provided as mb.Polymer

Exposing Tunable Chemistry as Simple Variables




```
pattern = Random2DPattern(100)
chain_length = 5
n_tiles = [2, 3, 1]
```

```
pattern = Grid2DPattern(5, 5)
chain_length = 20
n_tiles = [1, 1, 1]
```

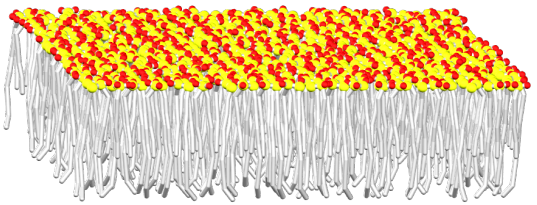
```
monolayer = AlkaneMonolayer(chain_length, pattern, n_tiles)
```

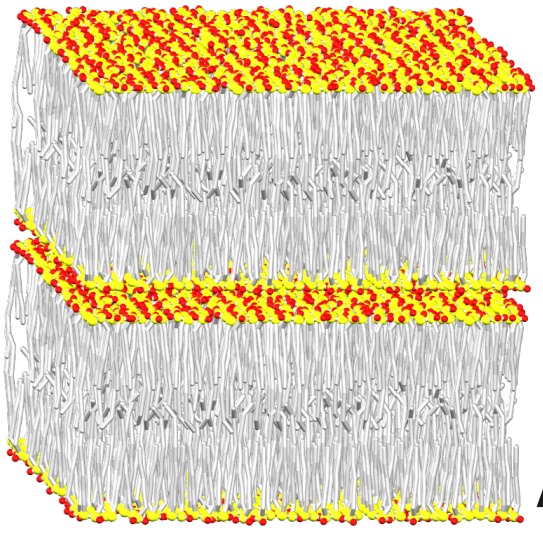

C. Klein, J. Sallai, T.J. Jones, C.R. Iacovella, C. McCabe, P.T. Cummings, A Hierarchical, Component Based Approach to Screening Properties of Soft Matter, in: Springer, Singapore, 2016: pp. 79–92. doi:10.1007/978-981-10-1128-3_5.

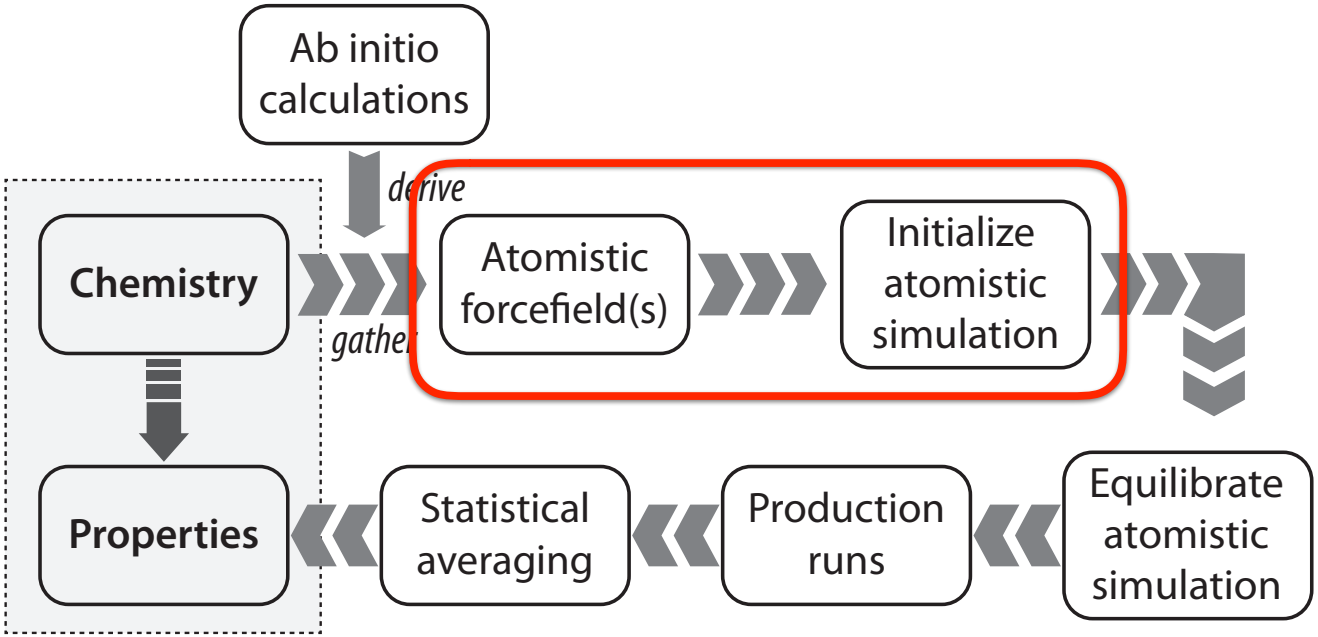
Using mBuild: CER Multilayer

- Easily build a ceramide multilayer with just a few lines of python
  - Read in molecule from pdb file
  - Build leaflet, then stack leaflets
  - 13 lines!

```
1  from numpy import pi
2  import mbuild as mb
3
4  cer2 = mb.load('cer2.pdb')
5  grid = mb.pattern.Grid2DPattern(50, 50)
6  leaflet, system = mb.Compound(), mb.Compound()
7  repeat_spacing = 6  # repeat spacing in nm
8  leaflet = grid.apply(cer2)  # put lipids on gird points
9  leaflet = mb.Compound(leaflet)
10 for layer_num in range(4):  # add 4 leaflets to the system
11     new_layer = mb.clone(leaflet)
12     if layer_num % 2 == 1:  # rotate every other layer 180deg
13         new_layer.spin(pi, around=[1, 0, 0])
14     new_layer.translate([0, 0, layer_num * repeat_spacing / 2])
15     system.add(new_layer)
16 system.save('cer2.hoomdxml')
```






Ab initio calculations
derive
Chemistry
Atomistic forcefield(s)
Initialize atomistic simulation
Properties
Statistical averaging
Production runs
Equilibrate atomistic simulation

Atom Typing and Applying Force Fields

- Need general purpose atom typer
  - Arbitrary chemistry means we cannot rely on templates
  - Needs to be easy to develop new atom types and associated logic
  - Don't want to rely on rigid rule hierarchies for atom type definitions
    - Ordered least to most general
- Removing gap between logic and parameters
  - Parameters exist in various files
  - Logic often encoded as series of if/else statements deep in source code
  - Why not combine the two?
- Similar concept being developed by Open Force Field group
  - https://github.com/open-forcefield-group/

Foyer: Applying and Disseminating force fields

- End user should only require
  - Force field file
  - Chemical topology

```
from foyer import Forcefield
import parmed as pmd

untyped_ethane = pmd.load_file('ethane.mol2', structure=True)
oplsaa = Forcefield(forcefield_files='oplsaa.xml')
ethane = oplsaa.apply(untyped_ethane)

# Save to any format supported by ParmEd
ethane.save('ethane.top')
ethane.save('ethane.gro')
```

Adding Atom Type Definitions to OpenMM XML

- OpenMM XML file convenient to extend
  - Existing infrastructure
  - Great support for custom functional forms

```
<ForceField>
 <AtomTypes>
  <Type name="opls_135" class="CT" element="C" mass="12.01100" def="[C;X4](C)(H)(H)H" desc="alkane CH3"/>
  <Type name="opls_140" class="HC" element="H" mass="1.00800"  def="H[C;X4]" desc="alkane H"/>
 </AtomTypes>
</ForceField>
```

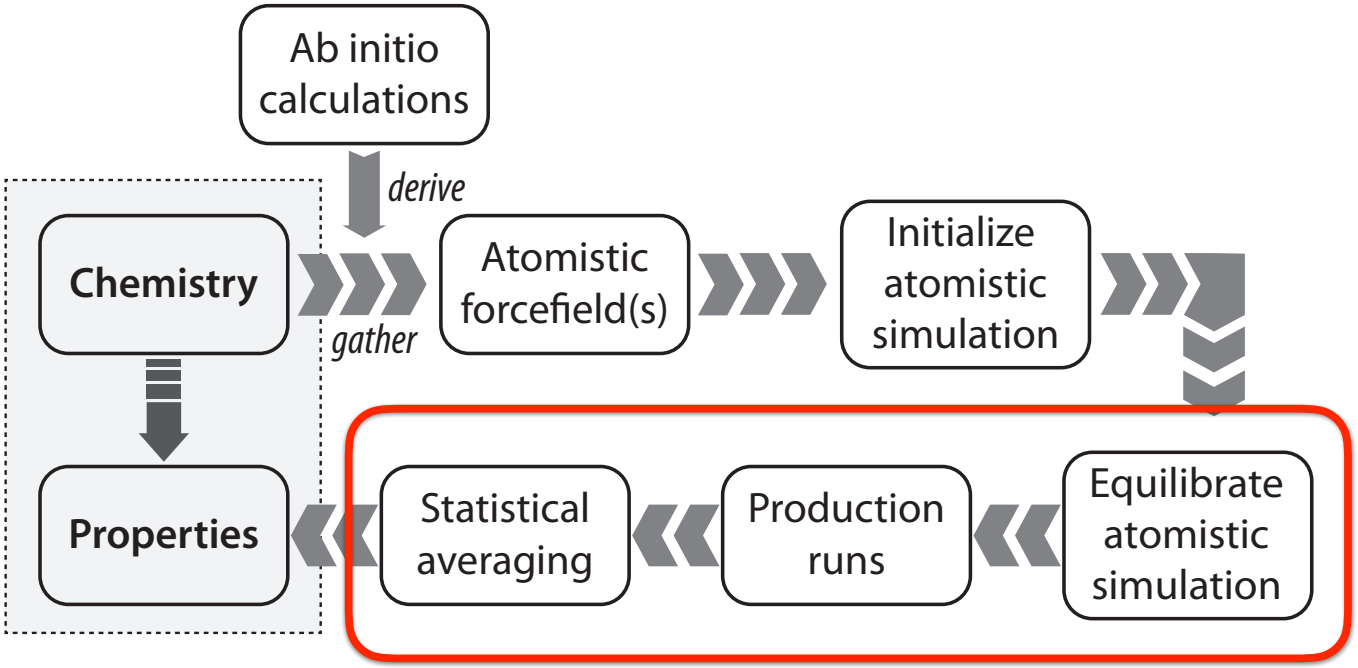
- Add machine/human readable SMARTS
  - First atom token in SMARTS indicates the type that we are defining
- Optionally, add colloquial description and DOI
  - Adding DOI produces BibTeX file when applying force field

Promoting Dissemination of Force Fields

- Template repo for building foyer compatible force field files
  - https://github.com/mosdef-hub/forcefield_template
  - Skeleton force field file
  - Skeleton testing setup
    - User needs to only add correctly typed .mol2 files
  - Tutorial for adding SMARTS definitions
    - Walkthrough for adding more and more complex definitions
    - Testing with small example set of hydro carbons from alkanes through alkenes and benzene
    - How to run tests with py.test and enable TravisCI for your repo
- Force field development within our group
  - **OPLS-AA compatible parameters for perfluoroethers**

    DOI 10.5281/zenodo.56807
  - Coarse-grained models for skin lipids
  - Automating force field derivation for supercapacitor electrodes

VANDERBILT


Ab initio calculations
derive
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MetaMDS - Overview

- MetaMDS was designed with the goal of being able to perform screening simulations
  - It can submit large batches of jobs with various input parameters
- MetaMDS relies on 3 key inputs:
  - mBuild "recipe"
    - This tells metaMDS how to construct the system
    - Allows us to screen over not just thermodynamic properties, but over different structures/molecules/etc.
  - Simulation template
    - This is a script that encapsulate the underlying simulation routines/calls
  - List(s) of parameters to vary
    - These parameters are used to change thermodynamic states in the simulation script and change inputs to the mBuild recipe
    - These lists could also include different forcefields to evaluate

MetaMDS - Screening

- By using simulation templates, mBuild recipes, and simple parameter lists, we can create a streamlined, abstracted interface
  - Users only need a few lines of code to do large scale, complex screening
  - Individual elements can be easily tested before large scale deployment
  - All procedures are well documented and described

In [ ]:
```
# Initialize a simulation instance with a template and some metadata
sim = mds.Simulation(name='monolayer', template=create_run_script, output_dir='output')

chain_lengths = [8, 12, 16, 20]
for length in chain_lengths:
    parameters = {'chain_length': length,
                  'n_molecules': 100,
                  'forcefield': 'OPLS-aa',
                  'build_func': build_monolayer}
    # Parameterize our simulation template
    sim.parametrize(**parameters)
```

In [ ]:
```
# Run
sim.execute_all(hostname='rahman.vuse.vanderbilt.edu', username='ctk3b')
```

In [ ]:
```
sim.sync_all()
```

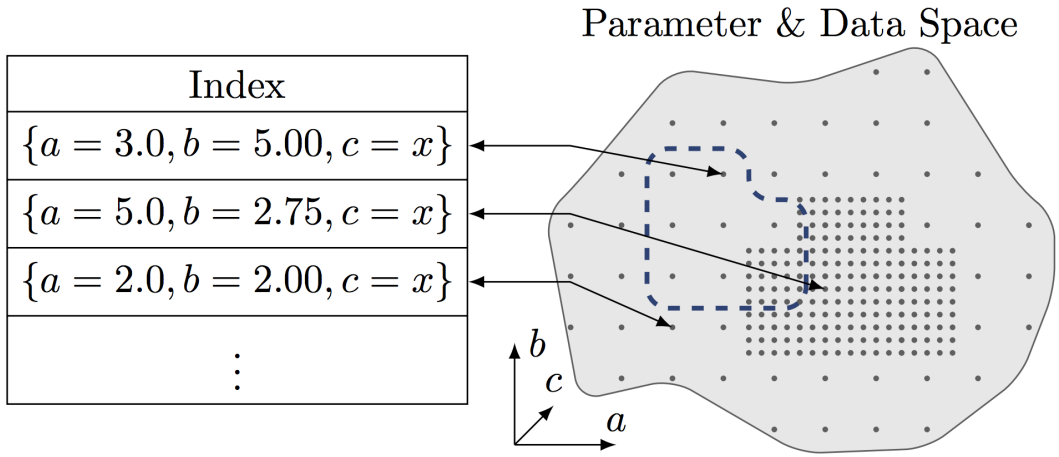

User interface is Python notebook (c.f. Mathematica)

MoSDeF

- Building a community
  - Hackathon in February with representation from 11 research groups and ExxonMobil
  - Goal of learning how to use MoSDeF and become co-developers
    - Add forcefields
      - *Currently support OPLS, TRAPPE, specific forcefields (e.g., ionic liquids)*
      - *Wish to add other standard forcefields (e.g., bio forcefields, ReaxFF generic and specialized) plus workflows to automate forcefield derivation*
    - Add simulation workflows for specific properties and applications
      - *Currently support many standard workflows, coarse-graining (MSIBI), etc*
      - *LONG wish list!*
    - Add simulation packages
      - *Currently support LAMMPS, GROMACS, HOOMD-Blue*
      - *Wish to add open-source AIMD codes, Monte Carlo (e.g., Cassandra), other MD codes*
  - Plan to jointly submit NSF SSI to support next MoSDeF cycle

Putting it All Together: Signac Workflow Manager

- Recently adopted in place of metaMDS
- Define heterogenous parameter spaces
- Provides link between data and metadata
  - Every job and its data is tied to a point in parameter space
  - Provides glue for seamless building, execution and analysis



Developed by Simon Adorf in Glotzer group

Adorf et al., arXiv:1611.03543 [cs.DB]

Putting It All Together

- Our tribology operations
  - mBuild + save with foyer
  - Minimize
  - Equilibrate
  - Shear at range of normal load
- Customize compute environment
  - Defaults provided for common envs
  - Collection of envs for major computing centers
    - OLCF, NERSC, NICS
- Execute and monitor

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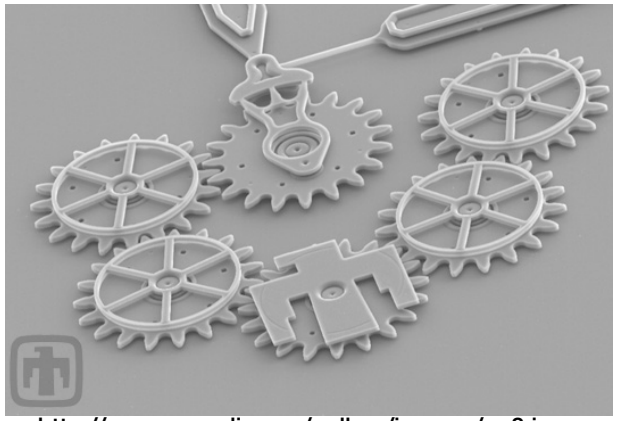
```
class MyTorqueEnvironment(flow.environment.TorqueEnvironment):
    hostname_pattern = 'mymoabcluster.university.edu'
    cores_per_node = 16

    @classmethod
    def mpi_cmd(cls, cmd, np):
        return 'mpirun -np {np} {cmd}'.format(n=np, cmd=cmd)

    @classmethod
    def script(cls, _id, nn, walltime, ppn=None, **kwargs):
        if ppn is None:
            ppn = cls.core_per_node
        js = super(MyTorqueEnvironment, cls).script()
        js.writeline('#!/bin/sh -l')
        js.writeline('#PBS -j oe')
        js.writeline('#PBS -l nodes={}:ppn={}'.format(nn, ppn))
        js.writeline('#PBS -l walltime={}'.format(format_timedelta(walltime)))
        js.writeline('#PBS -q low')
        js.writeline('#PBS -N {}'.format(_id))
        js.writeline('#PBS -V')
        return js
```

```
>>> project = MyProject()
>>> project.print_status(detailed=True, params=('a',))
Status project 'test-project':
Total # of jobs: 10
label         progress
------------  ------------------------------------------------
initialized   |######################################| 100.00%
processed     |########################--------------| 66.67%
Detailed view:
job_id                           S  next_job  a  labels
-------------------------------- -  --------  -  -------------------------
108ef78ec381244447a108f931fe80db U            1  initialized, processed
be01a9fd6b3044cf12c4a83ee9612f84 U            2  initialized, processed
32764c28ef130baefebeba76a158ac4e U  process   3  initialized
# ...
>>>
```

Intro to Nanotribology

- Micro- and nano-electromechanical devices (MEMS and NEMS) used in a wide range of applications
  - Accelerometers
    - Airbag deployment
    - Consumer electronics
      - *Apple iPhone, Nintendo Wii*
  - Micromirror arrays
    - HD projectors (DLP TV)
  - Sensors
- Typically applications avoid parts in contact
  - Surface forces such as adhesion, stiction, friction, and wear dominate
- Lubrication schemes needed for devices to reach full potential

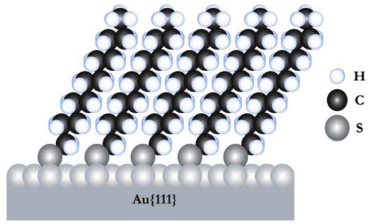


http://mems.sandia.gov/gallery/images/gc8.jpg

Monolayer Lubricants

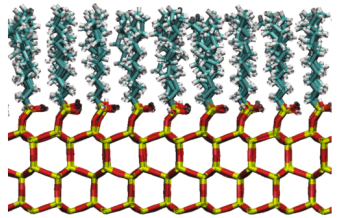
- Considerations for nanoscale lubricants
  - Low surface energy
    - **Minimize adhesion**
  - Low friction coefficient (μ)
    - **Minimize friction**
  - Robust/durable
    - **Wear-resistant**
- Alkylsilane monolayers
  - Densely-packed chains reduce surface energy, protect underlying surface from wear
    - Low adhesion between surfaces even in the presence of water
  - Friction coefficients vary widely by composition, density, and chain length
    - μ reduced to < 50% of value for bare silica[1]
  - Durability concerns

Alkanethiol monolayer on gold



Smith et al., *Prog. in Surf. Sci.*, 2004

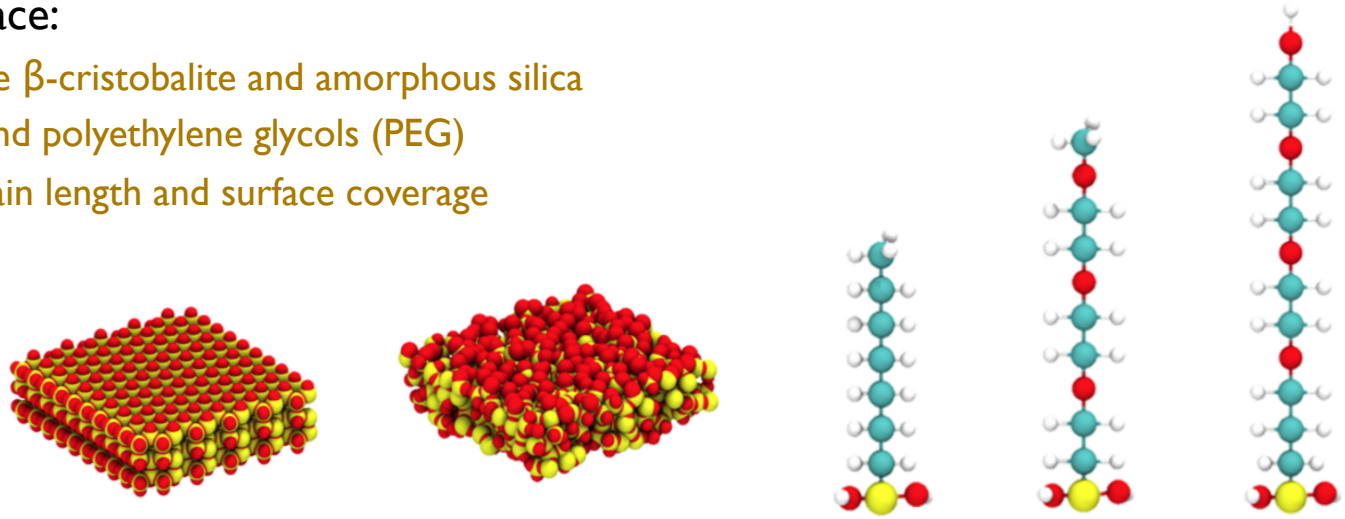
Alkylsilane monolayer on silica



Booth et al., *Langmuir*, 2011

Screening Monolayers (with metaMDS)

- Proposed hypotheses in the literature
  - More flexible chains reduce friction force on amorphous substrates
  - Crystalline monolayers imposed artificially induced ordering
    - Leads to lower friction coefficients
- Design space:
  - Crystalline β-cristobalite and amorphous silica
  - Alkanes and polyethylene glycols (PEG)
  - Varied chain length and surface coverage



Klein, C., Sallai, J., **Jones, T. J.**, Iacovella, C. R., McCabe, C. Cummings, P.T., "A Hierarchical, Component Based Approach to Screening Properties of Soft Matter," In Foundations of Molecular Modeling and Simulation: Select Papers from FOMMS 2015; R. Q. Snurr; C. S. Adjiman and D.A. Kofke, Ed.; Springer Singapore: Singapore, 2016; pp 79-92.

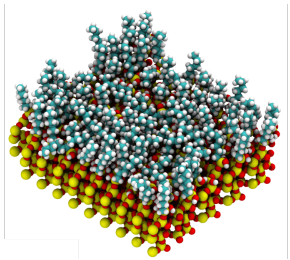
Nematic Order

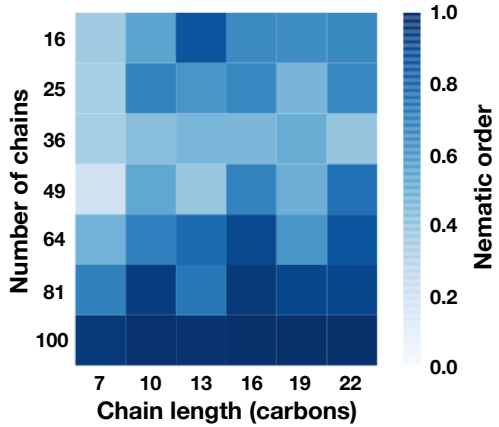
- **Nematic order** - measure of the global orientational ordering of monolayer chains
  - 0 = isotropic
  - 1 = perfectly ordered

$$S_2 = \langle \frac{3}{2}\cos^2\theta - \frac{1}{2} \rangle$$

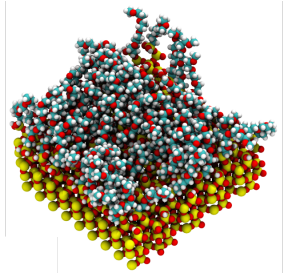
- PEG is found to feature lower nematic order than alkanes, particularly at lower surface coverage
  - Floppier/more liquid-like

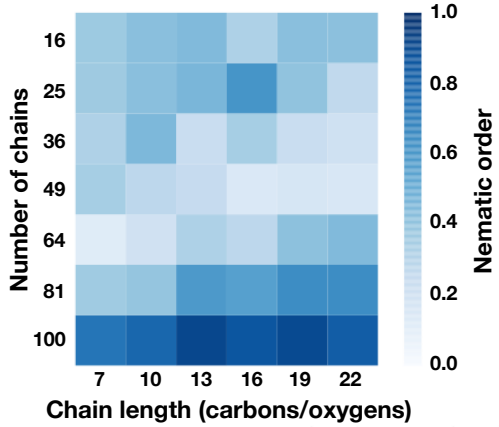
Alkanes





PEG





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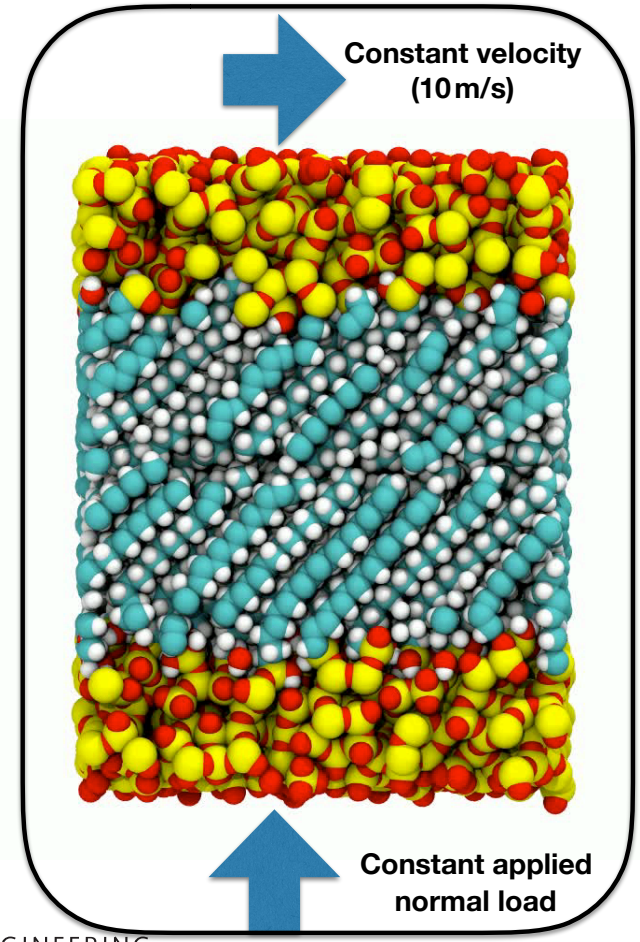
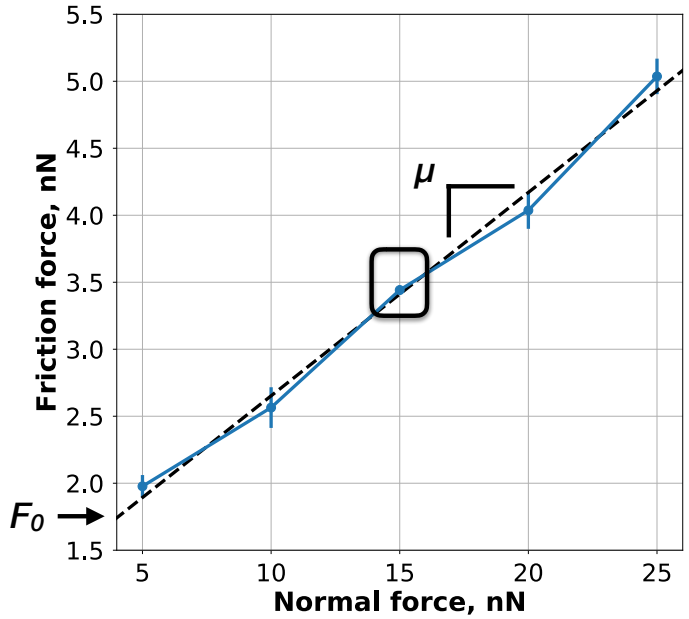
Evaluating Lubricity

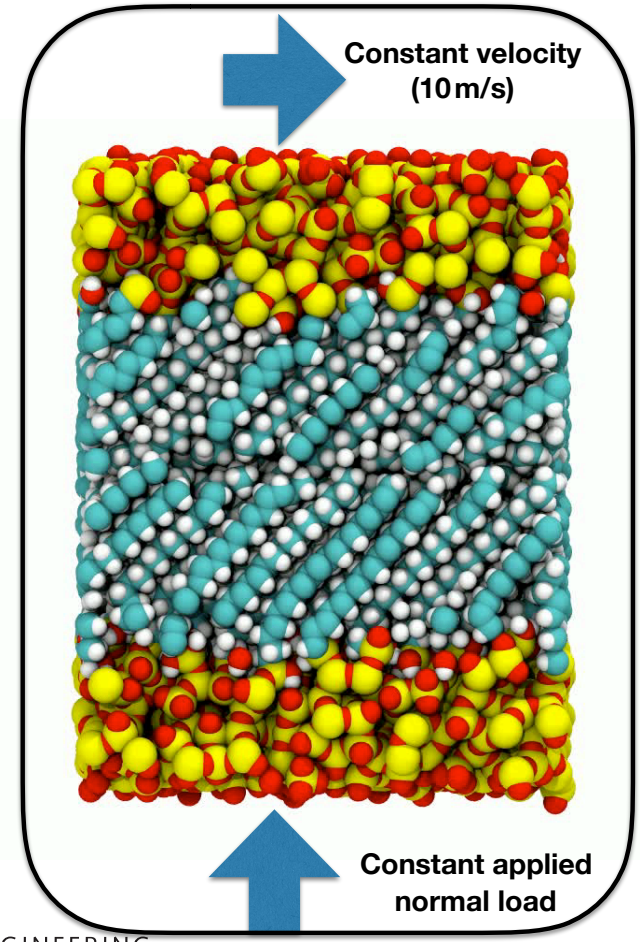


Derjaguin form of Amonton's Law of Friction

$$F_{\text{friction}} = F_0 + \mu F_{\text{normal}}$$



Evaluating Lubricity



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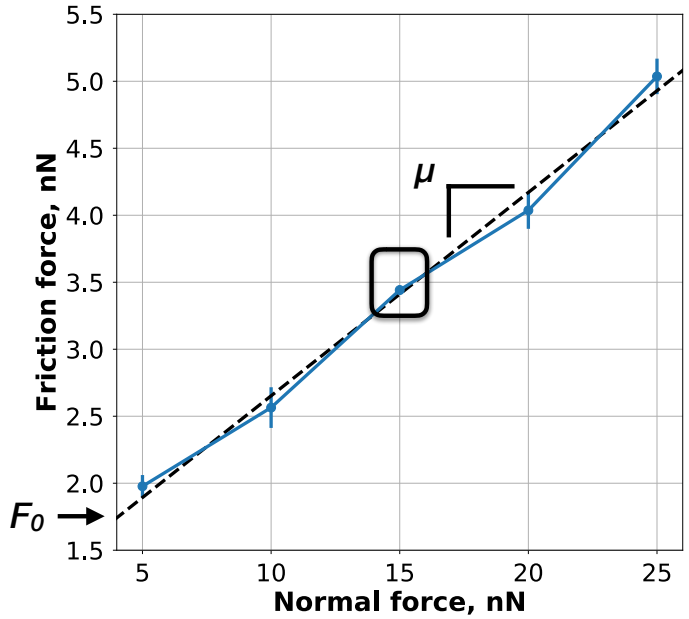
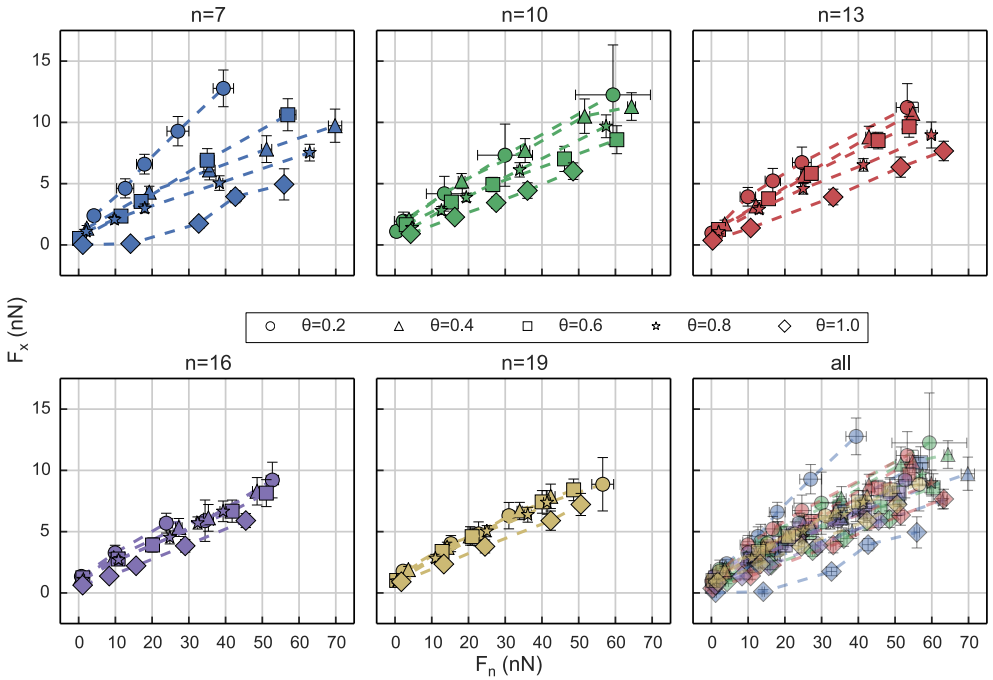


Surface Coverage has Greater Impact on Short Chains

- Subset of friction force data for polyethylene glycol monolayers on crystalline surface



- n = number of C/O atoms in chain
- θ = fractional surface coverage

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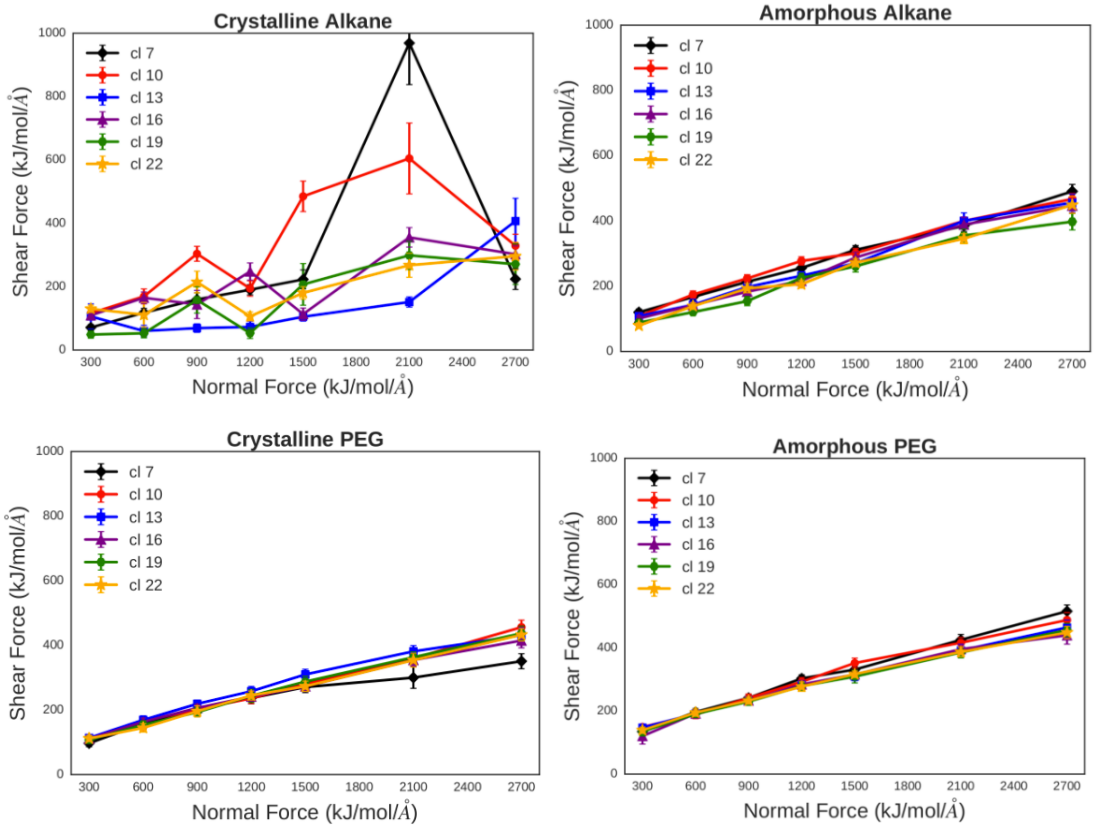
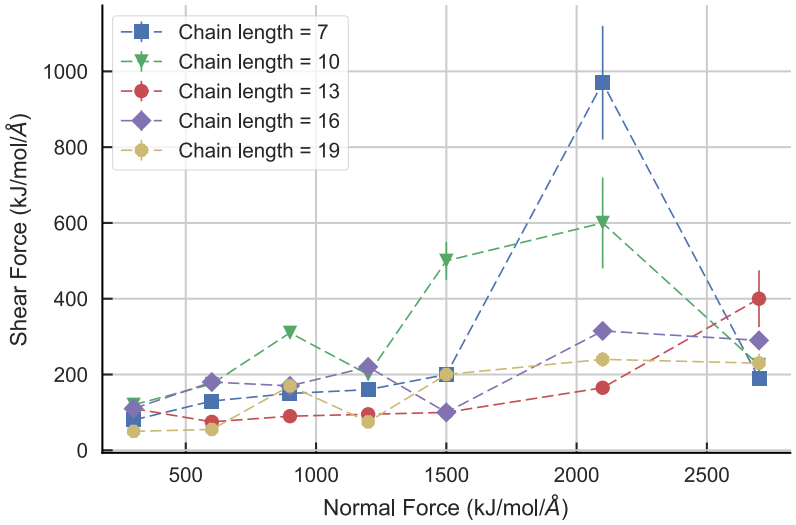
Friction Forces

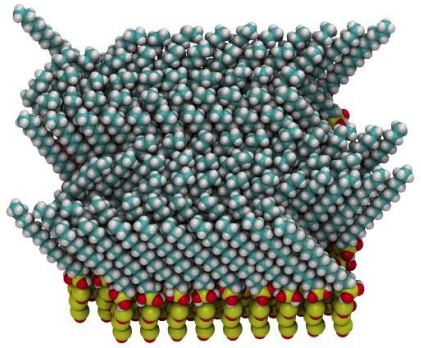
- Similar behavior for PEG and alkanes on amorphous surface
- Strange results for alkanes on crystalline surfaces



Crystalline Monolayers Can Exhibit artifacts

- Crystalline monolayers impose artificial ordering on monolayers
  - Portions of monolayer can get trapped in different configurations
  - High forces perpendicular to shear direction





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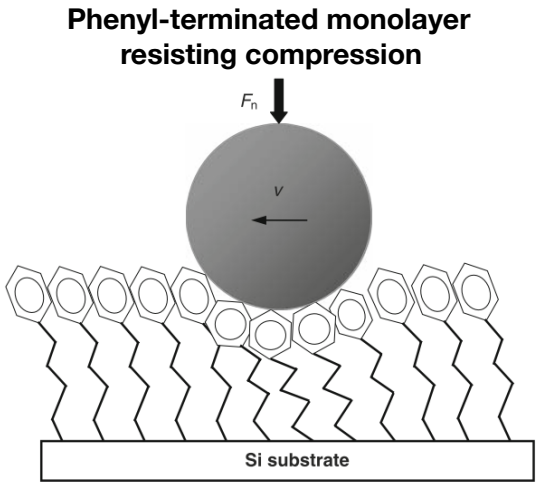
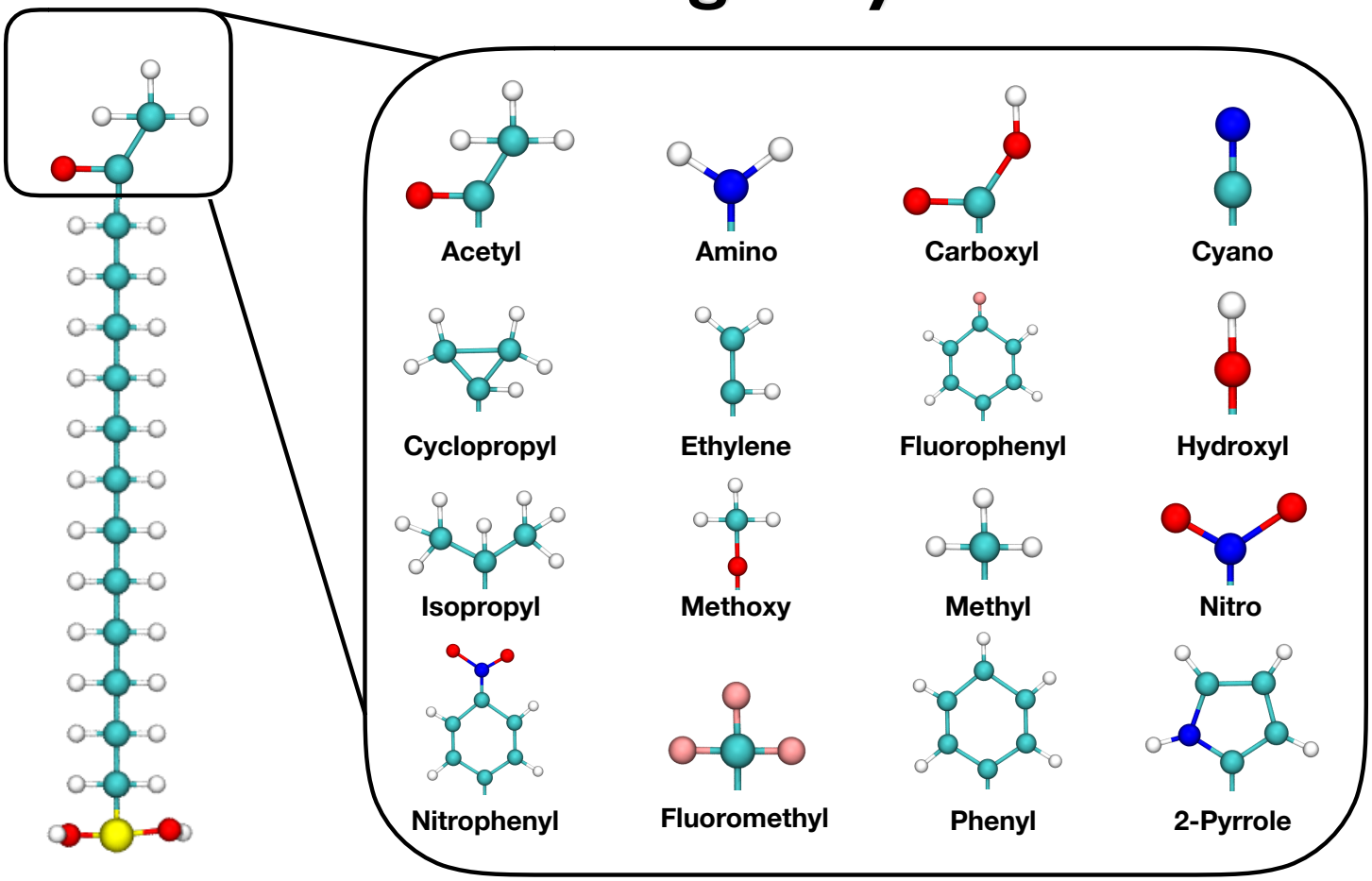
Terminal Group Chemistry

- Terminal groups form the boundary at the monolayer interface, thus having important effects on tribology
  - Methyl most common - low surface energy
- Higher friction forces in hydroxyl-terminated monolayers
  - Attributed to H-bonding across the monolayer interface
- Phenyl terminal groups can improve durability by resisting asperity penetration
- Only a few chemistries studied in the context of lubrication

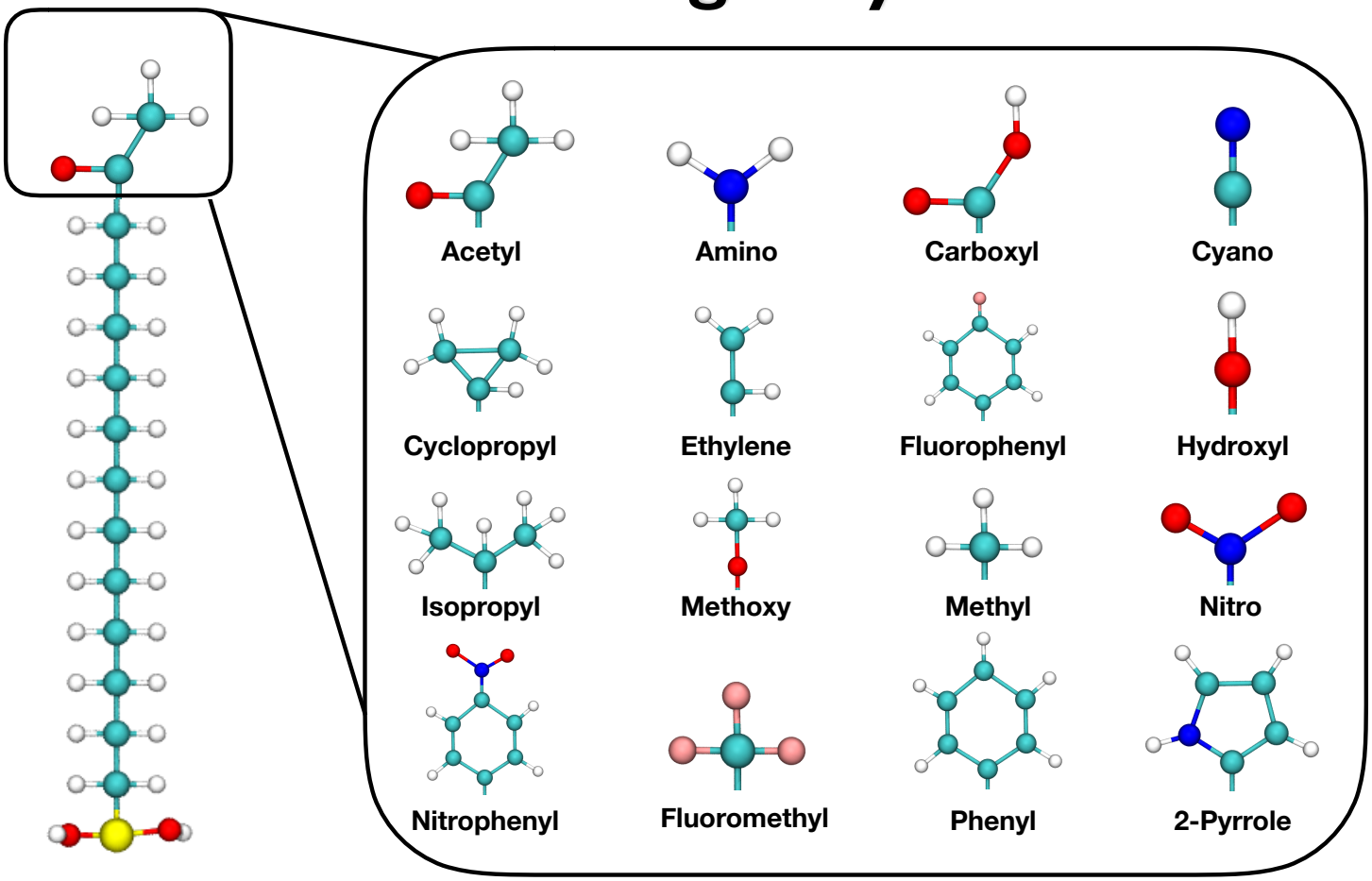


Yu et al., *Tribol. Lett.*, 2009

Constructing Alkylsilanes

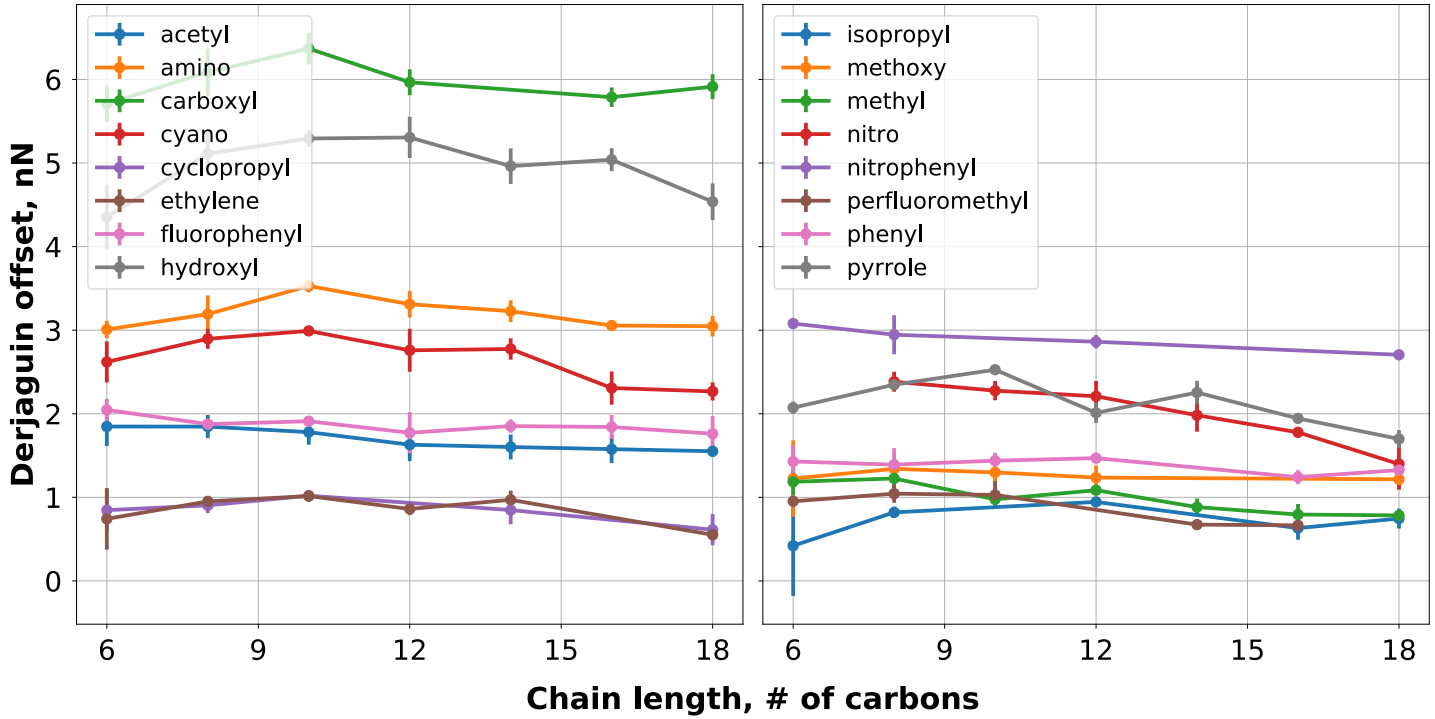


Constructing Alkylsilanes



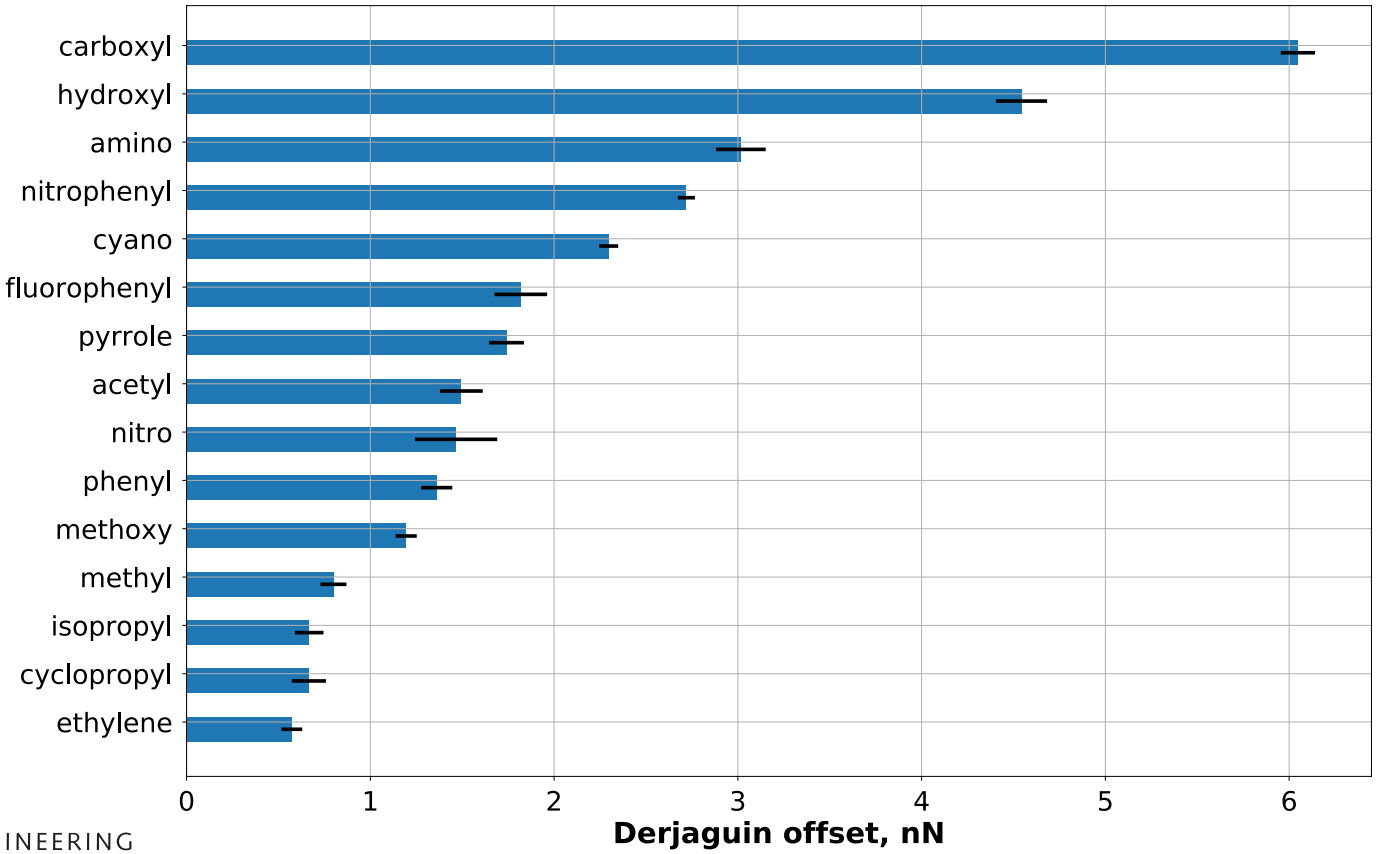
Derjaguin Offset

$$F_{\text{friction}} = \boxed{F_0} + \mu F_{\text{normal}}$$



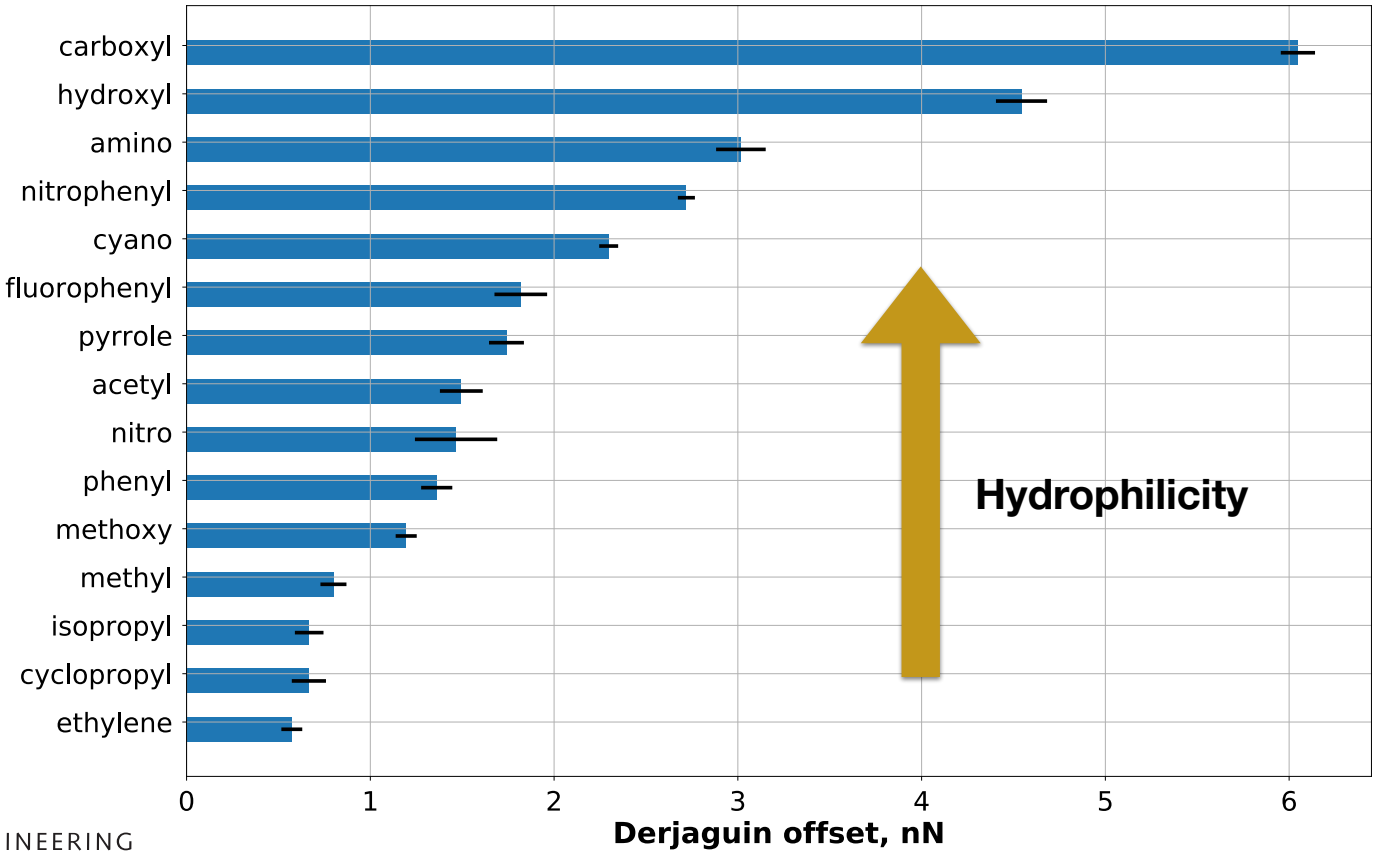
Derjaguin Offset (C18)

$$F_{\text{friction}} = \boxed{F_0} + \mu F_{\text{normal}}$$



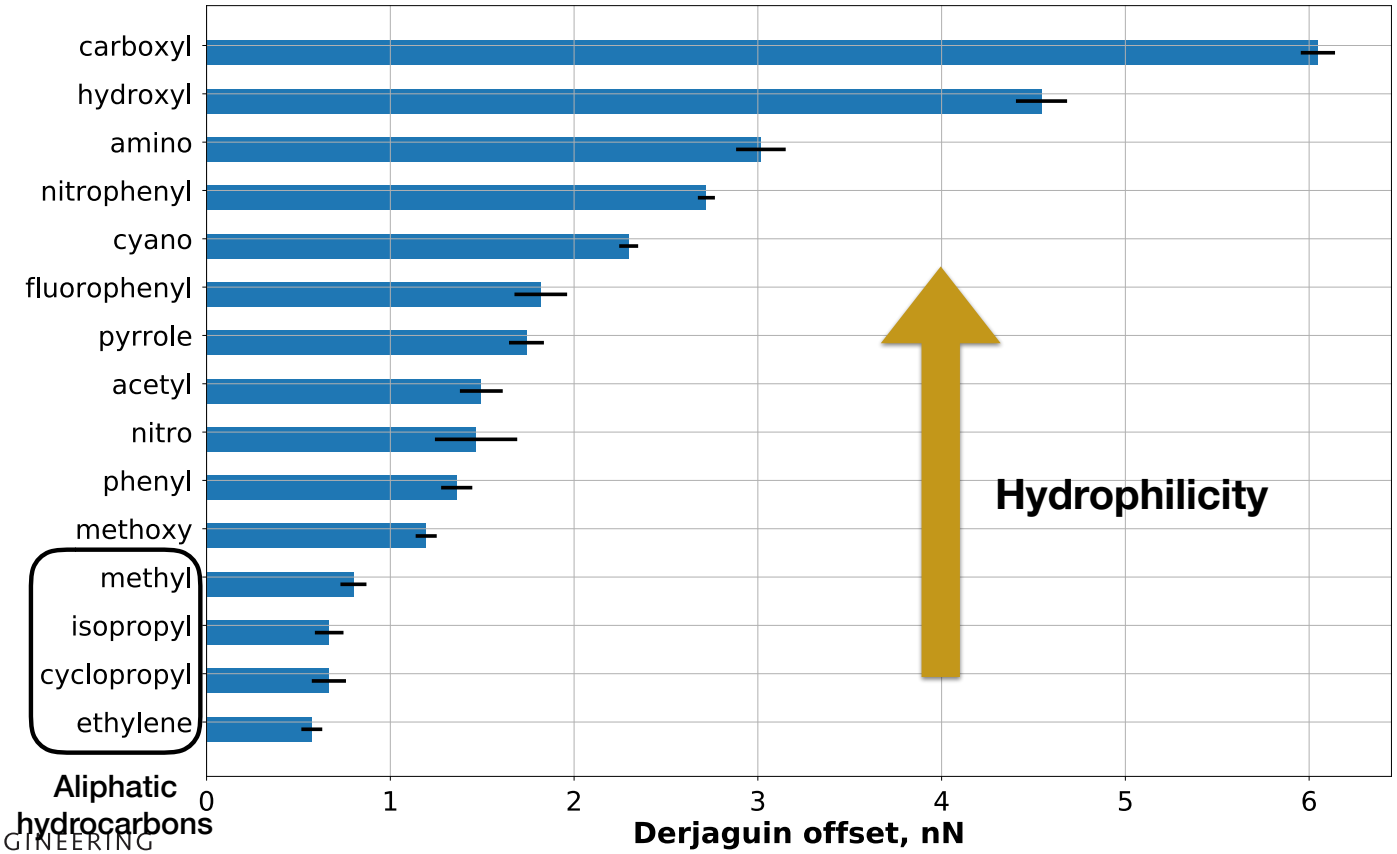
Derjaguin Offset (C18)

$$F_{\text{friction}} = \boxed{F_0} + \mu F_{\text{normal}}$$



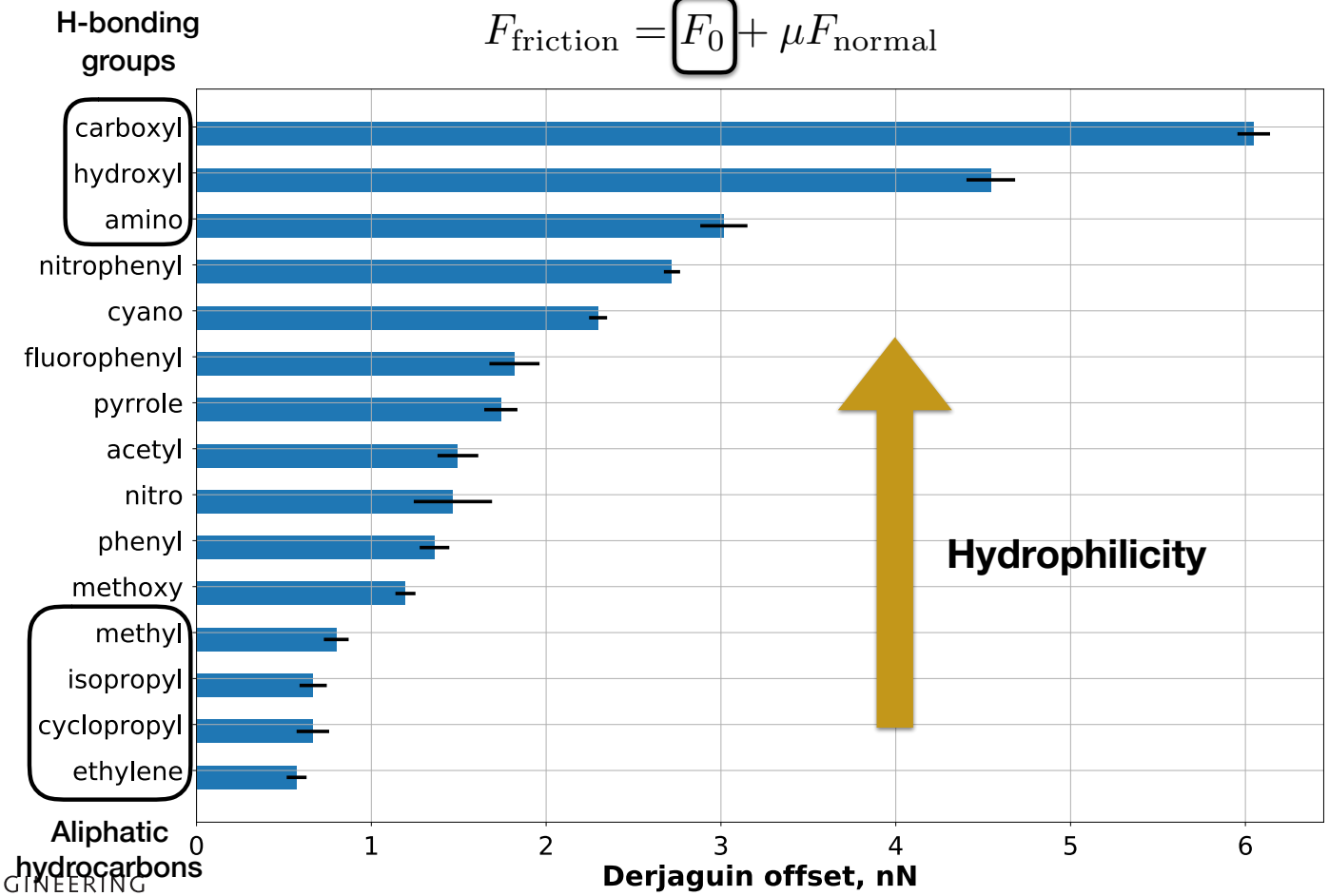
Derjaguin offset (C18)

$$F_{\text{friction}} = F_0 + \mu F_{\text{normal}}$$

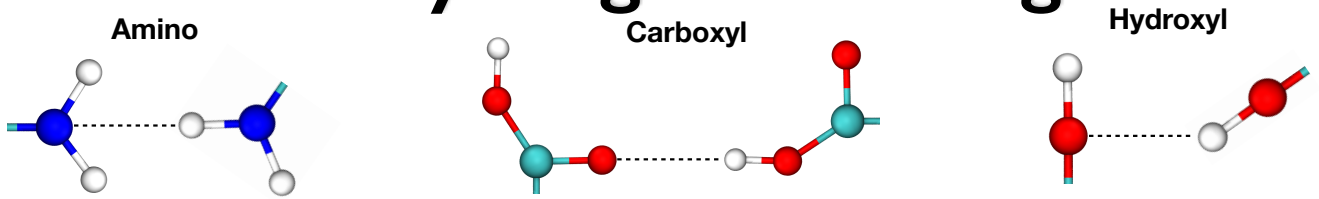


Derjaguin Offset (C18)

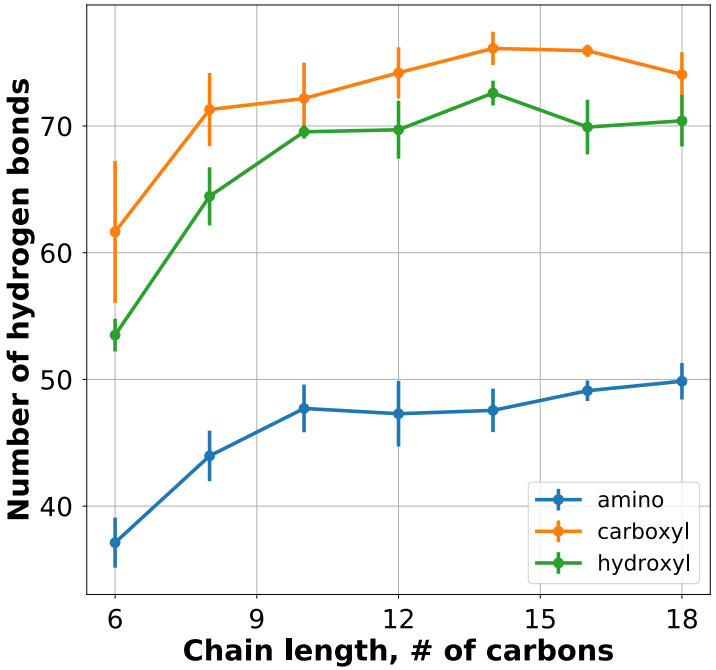
$$F_{\text{friction}} = F_0 + \mu F_{\text{normal}}$$



Hydrogen Bonding



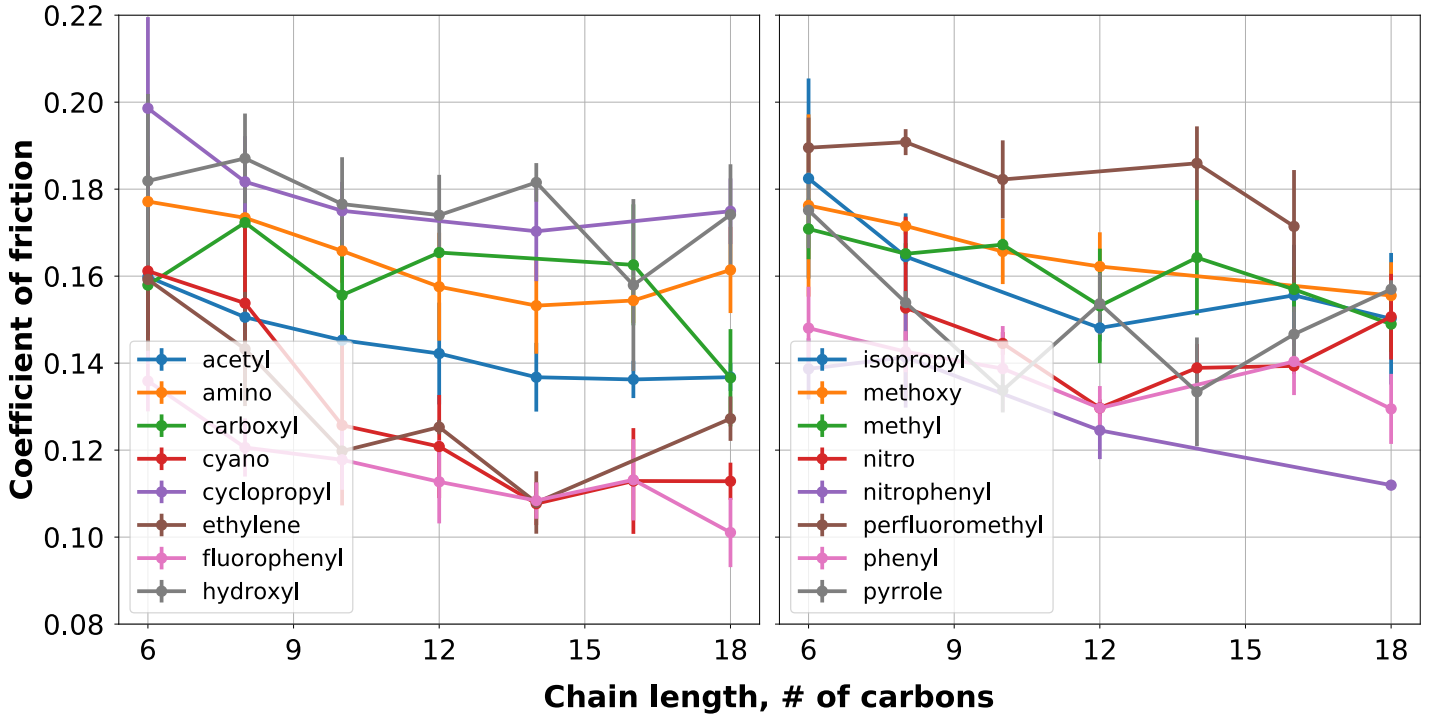
- $n_{amino} < n_{hydroxyl} < n_{carboxyl}$
  - Number of H-bonds determined using the Wernet-Nilsson method*
- Agrees with trends in Derjaguin offset - following expectations from the literature
- Number of H-bonds increases as backbone length increases from 6 to 10 carbons
  - Likely a result of increased orientational order of chains



*Wernet et al., *Science*, 2004

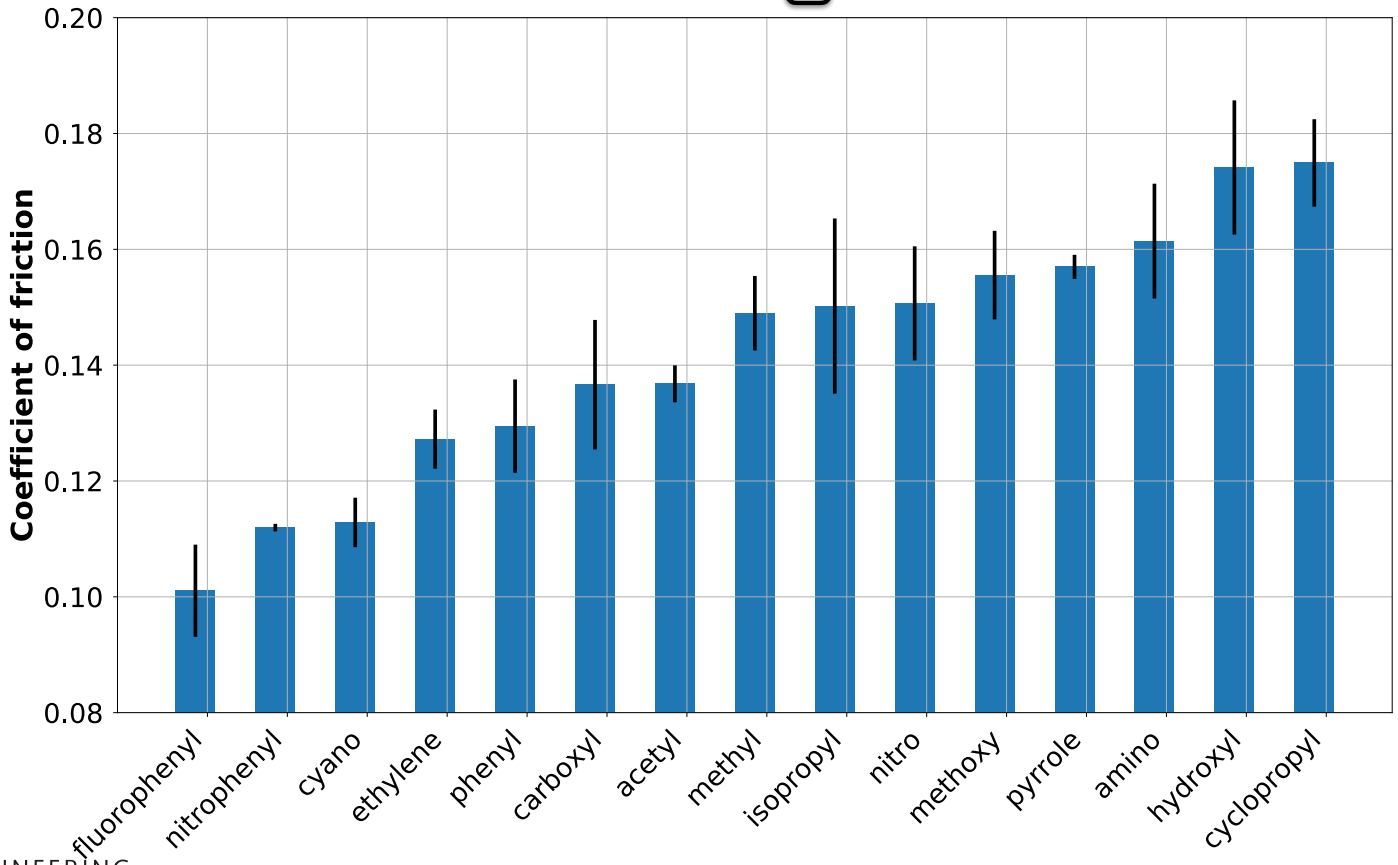
Coefficient of Friction

$$F_{\text{friction}} = F_0 + \mu F_{\text{normal}}$$



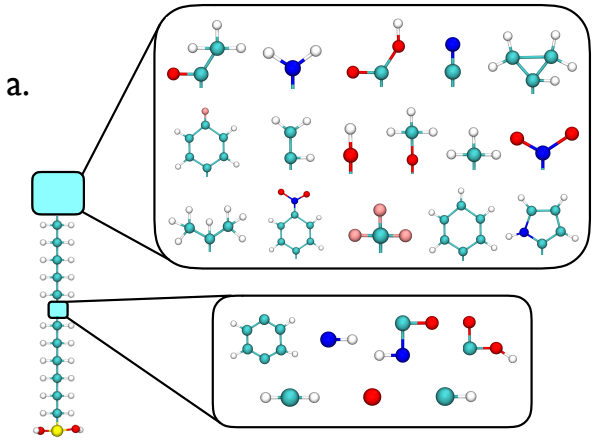
Coefficient of Friction - C18

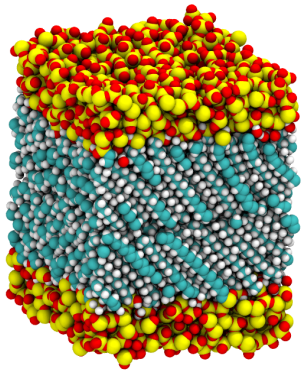
$$F_{\text{friction}} = F_0 + \mu F_{\text{normal}}$$



Next Steps

- Large parameter set screening
  - Other factors which affect tribological behavior
    - Different tether chemistry
    - Mixed monolayers
      - *Mixed length, end-functionalization, tether chemistry*
    - Asymmetric functionalization - different end groups on tethers
      - *For N ways to produce a monolayer, N(N+1)/2 asymmetric functionalization scenarios*
    - Identified ~45,000 variations to be screened
      - *Hope to perform on OLCF Titan in the next few months*





Conclusions

- To perform MGI-style screening of soft materials requires automating many steps currently largely performed by hand
- MoSDeF is an environment for automating molecular simulations
  - mBuild, Foyer, metaMDS,….
- Simulations performed within MoSDeF are completely reproducible
  - All steps are scripted, which can be distributed online through github
    - In line with identified best practices for reproducibility of computational research
- MoSDeF is being co-developed with other groups interested in transparency, reproducibility, usability, and extensibility (TRUE)
- Application to nanoscale lubrication is one example of application of soft materials screening made possible by MoSDeF and other tools (Signac)
- All resources available on github with version control
  - MoSDeF Hub - https://github.com/mosdef-hub
  - Foyer - https://github.com/mosdef-hub/foyer and mBuild - https://github.com/mosdef-hub/mbuild

Acknowledgments

- VU ChBE
  - Clare McCabe
  - Chris Iacovella
  - Christoph Klein
  - Andrew Summers
  - Justin Gilmer
  - Trevor Jones
- VU ISIS
  - Akos Ledezci
  - Gabor Karsai
  - Janos Sallai
  - Tengyu Ma

- Funding
  - NSF ACI 1047828: Development of an Integrated Molecular Design Environment for Lubrication Systems (iMoDELS)
  - NSF CDI CBET 1028374: Cyber-Enabled Design of Functional Nanomaterials
  - NSF SSE ACI 1535150: Development of a Software Framework for Formalizing Forcefield Atom-Typing for Molecular Simulation
- Resources
  - National Energy Research Supercomputing Center (NERSC), Lawrence Berekeley Laboratory
  - Oak Ridge Leadership Class (OLC), Oak Ridge National Laboratory