Multimode Propellant Discovery: A Computational High-throughput Screening Paradigm

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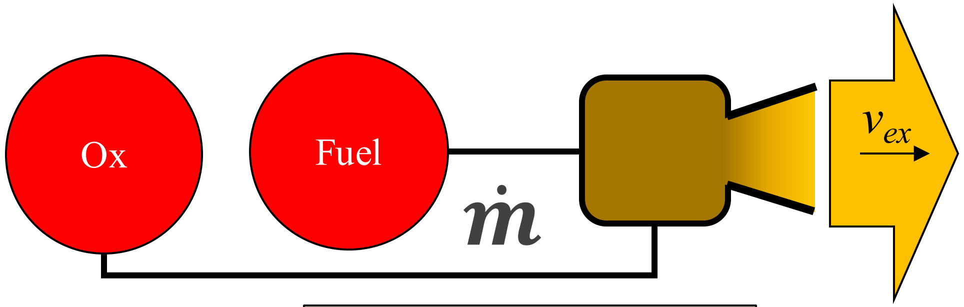
IEPC 2024, ID: 756

Motivation: Multimode Propulsion

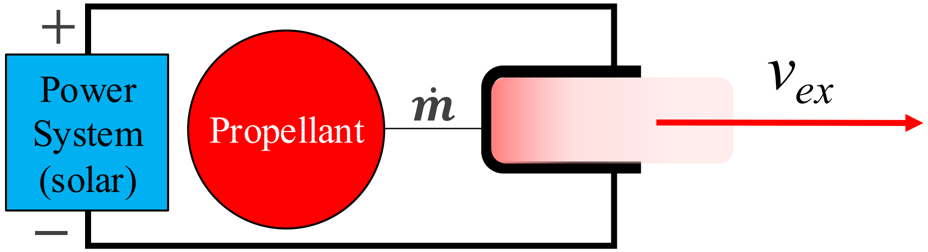
Multimode Propulsion (MMP) Overview

Chemical Propulsion



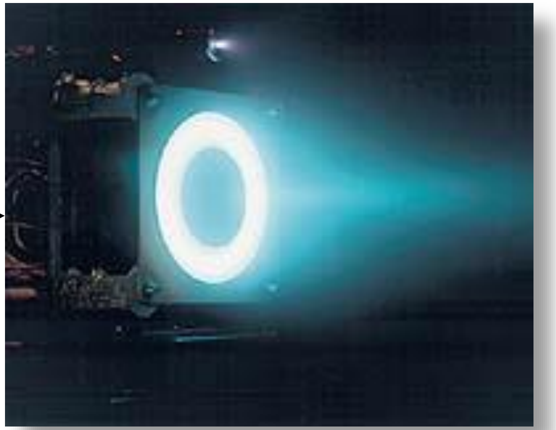
$T \cong 1$ N – MN+

Electrostatic EP*



$T \cong 0.1$ – 100's mN

Images: NASA, ESA



*Target Isp > 1000 s

D.C. Byers, J.W. Dankanich, Geosynchronous-earth-orbit communication satellite deliveries with integrated electric propulsion, *J. Propul. Power* 24 (6) (2008).

Multimode Propulsion (MMP) Overview

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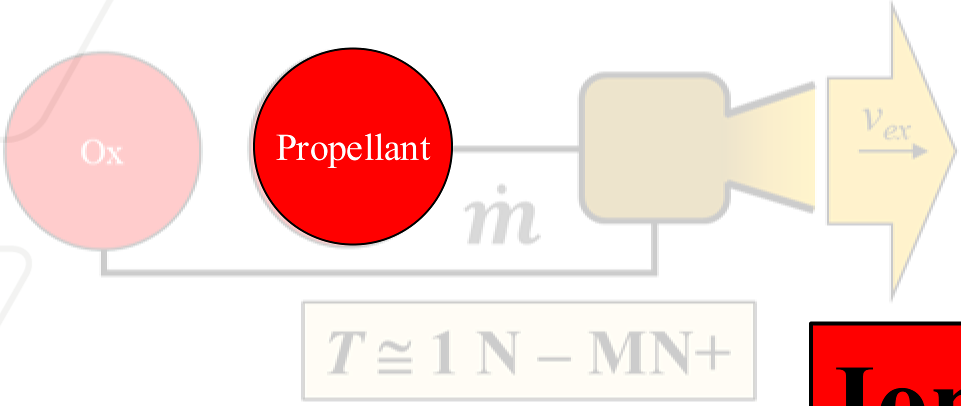
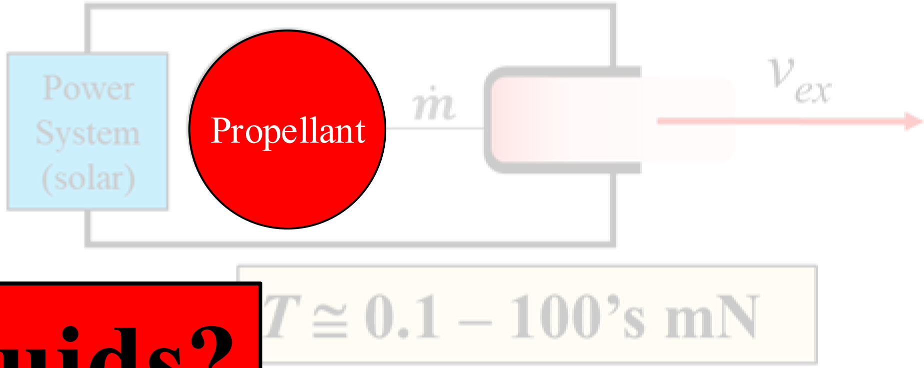


Electric Propulsion

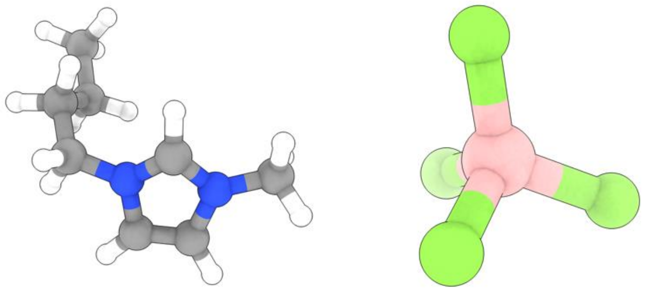


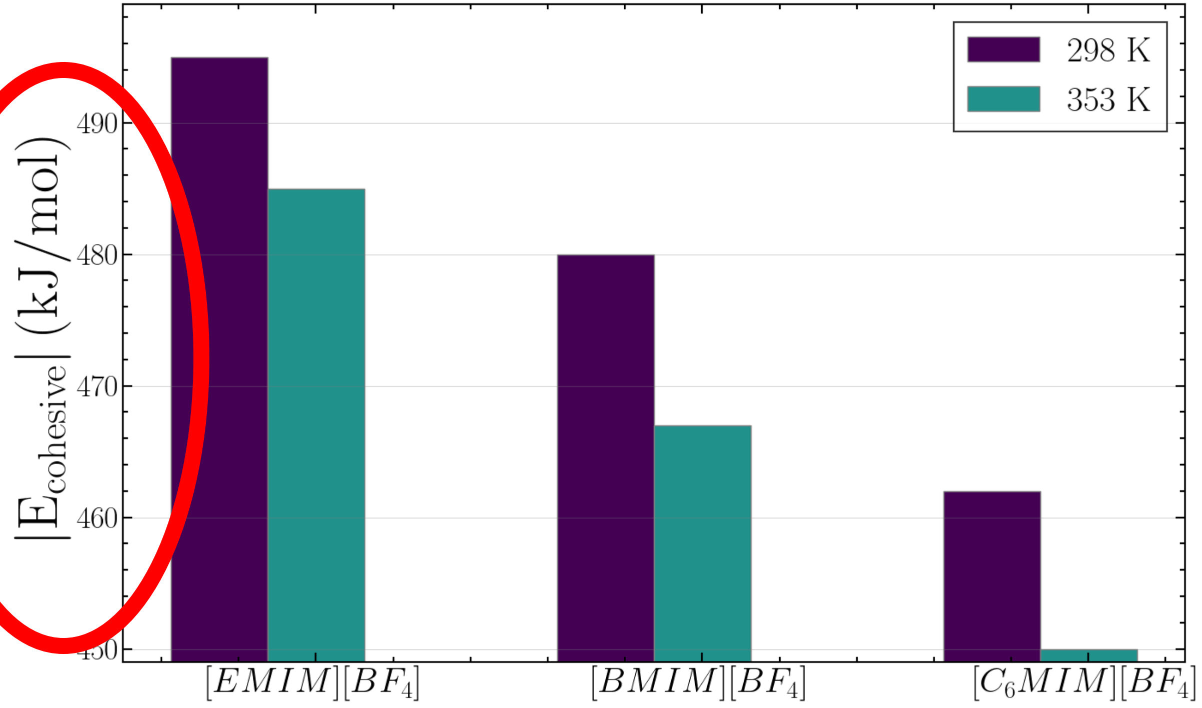
Ionic liquids?

~~Hydrazine~~

~~Argon~~
~~Krypton~~
~~Xenon~~
~~Iodine~~

What are Ionic Liquids (ILs)?

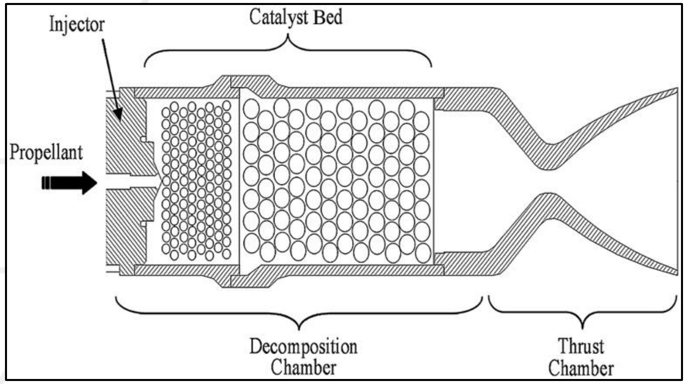


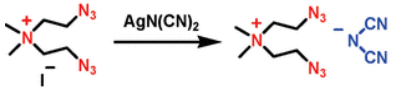


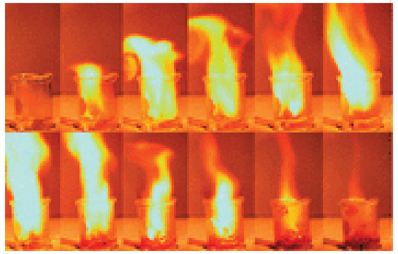
- Room-temperature molten salts
- Strong Coulombic attraction → **large cohesive energies**
- Favorable properties like…
  - Low vapor pressures
  - High electrical conductivities
  - Wide electrochemical windows
  - Tunability
  - …and many more!

Ionic Liquid-based Propulsion Systems

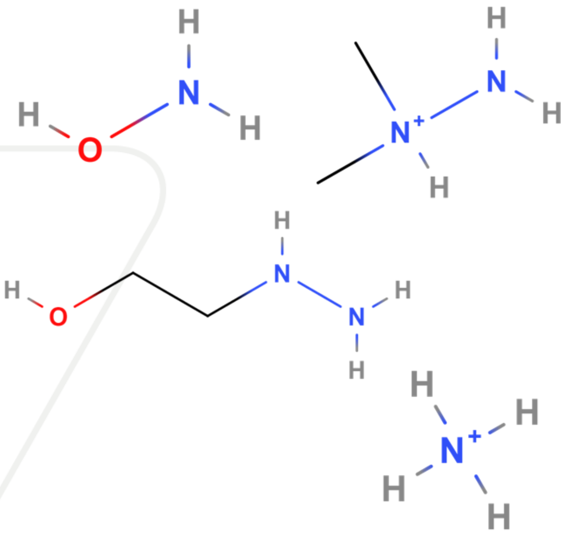
Chemical propulsion



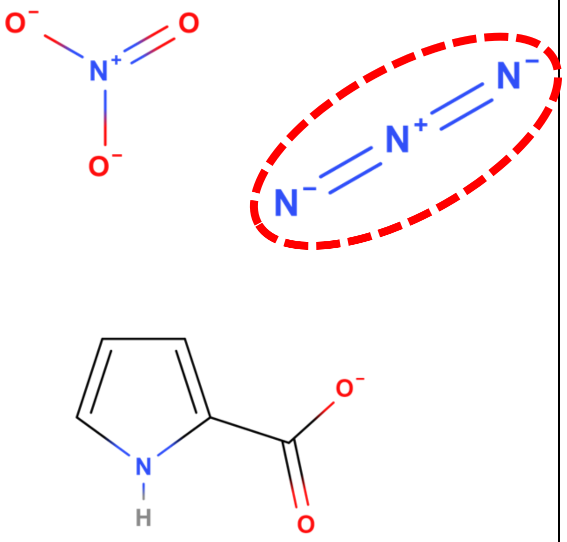




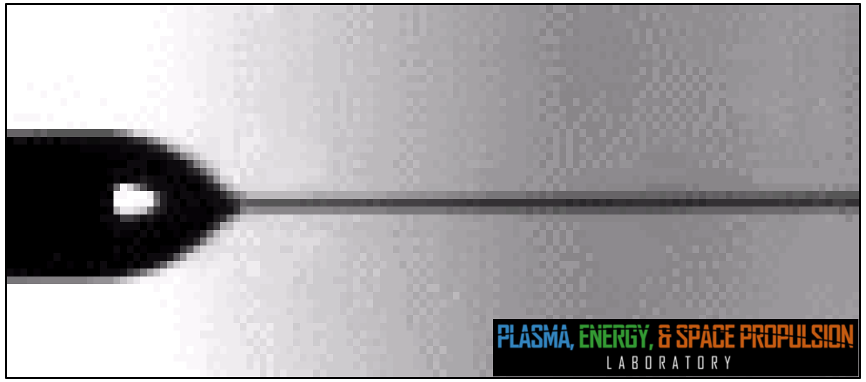
Cations



Anions



Electric Propulsion



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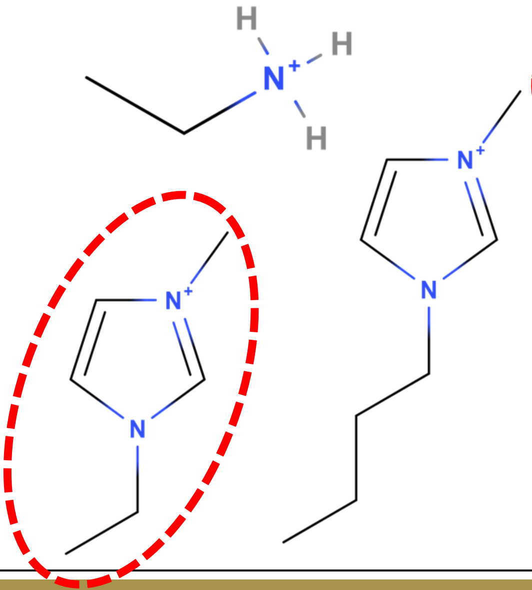

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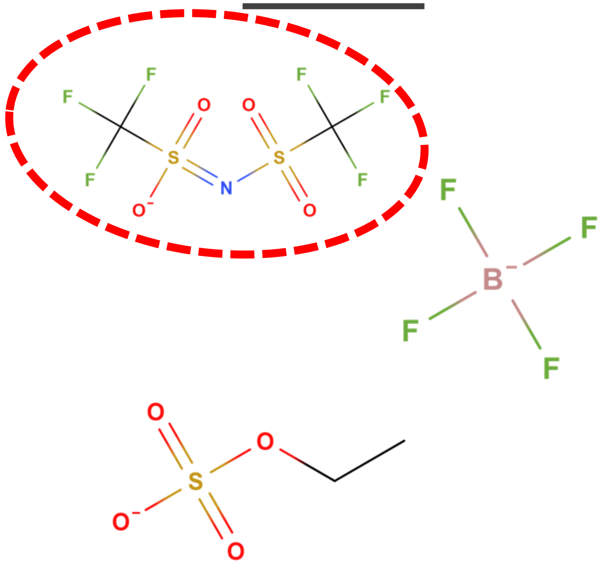
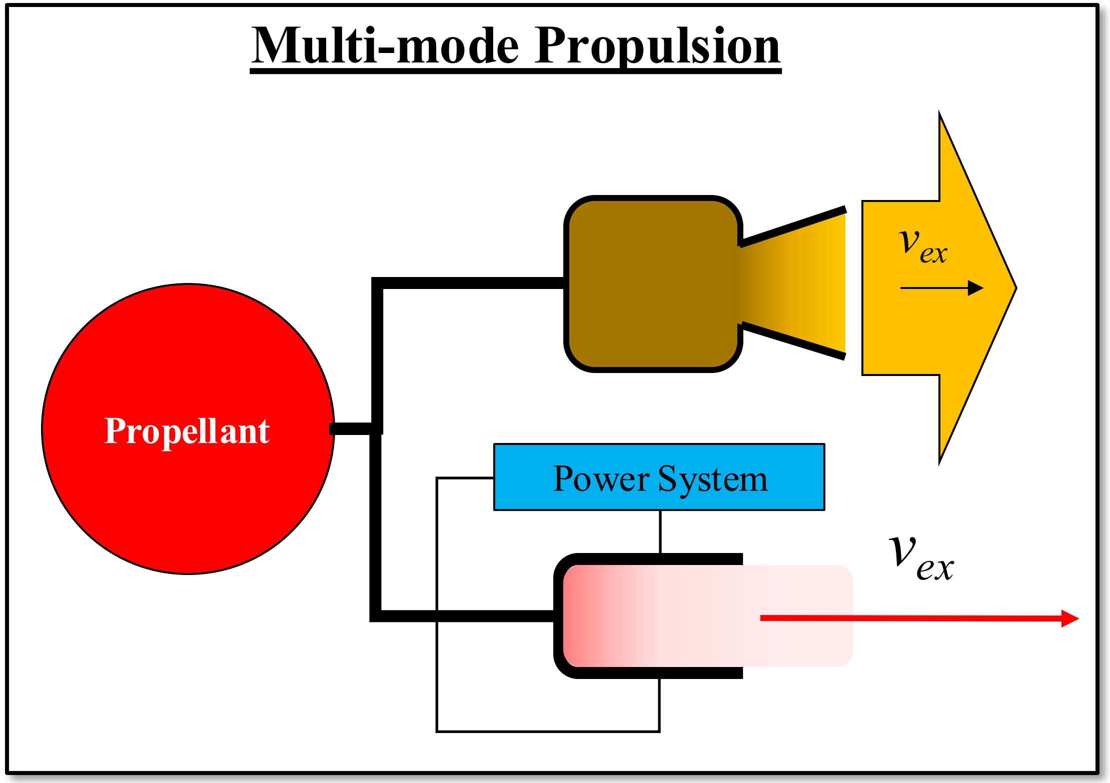


Multimode Propulsion: One propellant to rule them all?



"The major current research challenge is compatibility between thruster and propellant technologies."

J. L. Rovey, C. T. Lyne, A. J. Mundahl, N. Rasmont, M. S. Glascock, M. J. Wainwright, and S. P. Berg, "Review of multimode space propulsion," *Progress in Aerospace Sciences*, vol. *118*, p. 100627, **2020**.

High Throughput Propellant Screening

MMP Propellant Screening

Ionic Liquid	Specific Conductivity [$S.m^{-1}$]	Surface Tension [$mN.m^{-1}$]	Dynamic Viscosity [mPA.s]	Electrospray Selection Metric ($\sqrt{\gamma\kappa}$)	Monopropellant Selection Metric $\left(\sqrt{\Delta H_d/\overline{W}}\right)$
[MMIm] [Tf_2N]	0.888	37.6	44.00	5.78	5.11×10^{-2}
[EMIm] [Tf_2N]	0.866	37.3	32.40	5.68	5.34×10^{-2}
[MA] [$(C_1)O_2$]	4.380	43.1	17.00	13.74	6.75×10^{-2}
[EA] [HSO_4]	0.440	56.3	128.00	4.98	5.85×10^{-2}
[EA] [NO_3]	2.550	48.8	32.00	11.15	6.14×10^{-2}
[PA] [NO_3]	0.983	40.7		6.32	6.92×10^{-2}
[DMA] [HSO_4]	0.810	69.5	120.00	7.5	5.84×10^{-2}
[EoA] [HSO_4]	0.490	82.1	309.00	6.34	5.62×10^{-2}
[EoA] [$(C_1)O_2$]	0.370	65.0	162.50	4.9	7.20×10^{-2}
[EoA] [NO_3]	0.935	50.6	113.00	6.88	5.76×10^{-2}
[22HEEA] [HSO_4]	0.032	57.7	1310.00	1.36	6.45×10^{-2}
[22HEEA] [NO_3]	0.112	61.8	281.00	2.63	6.87×10^{-2}
[AlaE] [NO_3]	0.038	46.7		1.33	6.63×10^{-2}
[HAN]					2.99×10^{-2}
[ADN]					2.95×10^{-2}

Ewan Fonda-Marsland and Charlie Ryan. "Preliminary Ionic Liquid Propellant Selection for Dual-Mode Micro-Propulsion Systems," AIAA 2017-5019. *53rd AIAA/SAE/ASEE Joint Propulsion Conference*. July 2017.

MMP Propellant Screening

Ionic Liquid	Specif Conduct [S.m
[MMIm] [Tf_2N]	0.88
[EMIm] [Tf_2N]	0.86
[MA] [$(C_1)O_2$]	4.38
[EA] [HSO_4]	0.44
[EA] [NO_3]	2.55
[PA] [NO_3]	0.98
[DMA] [HSO_4]	0.81
[EoA] [HSO_4]	0.49
[EoA] [$(C_1)O_2$]	0.37
[EoA] [NO_3]	0.93
[22HEEA] [HSO_4]	0.03
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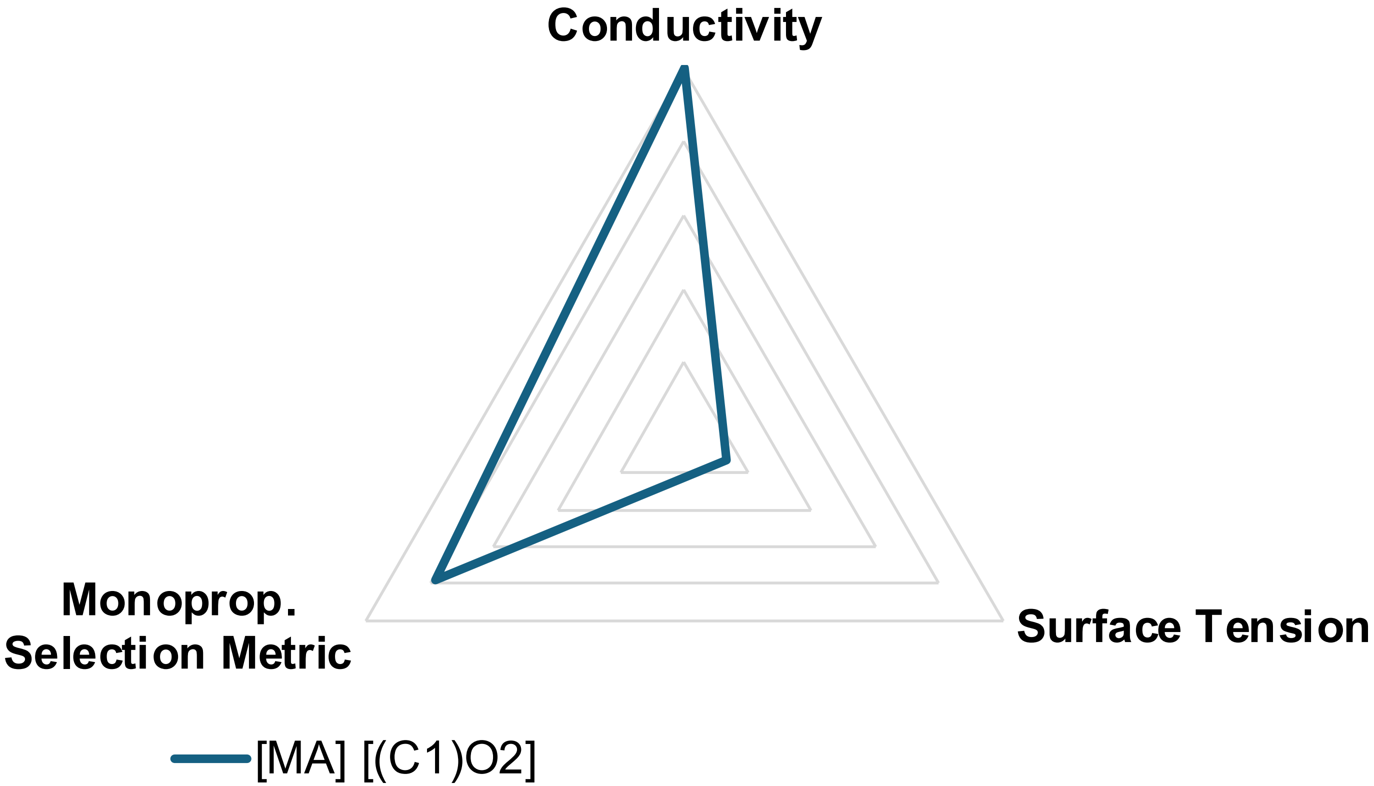
[ADN]	



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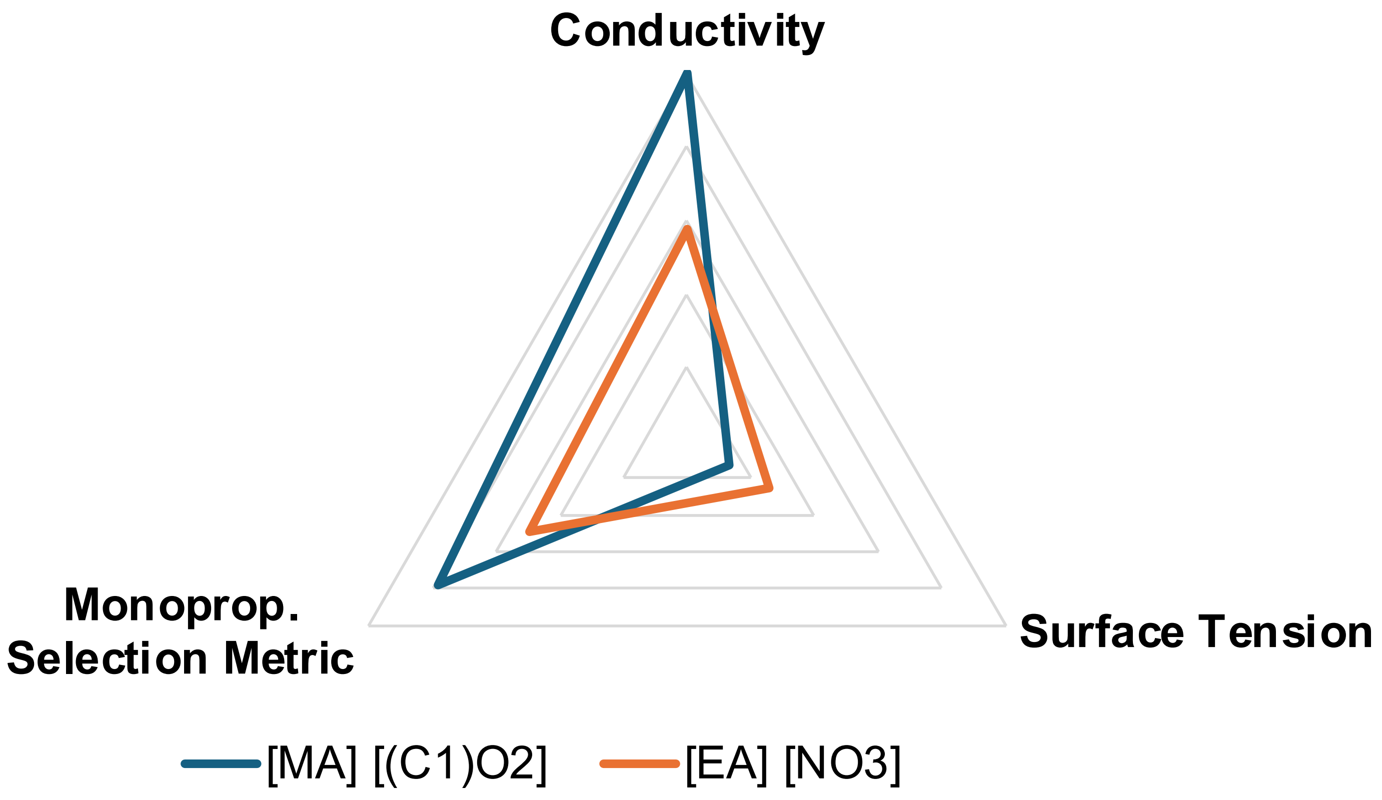

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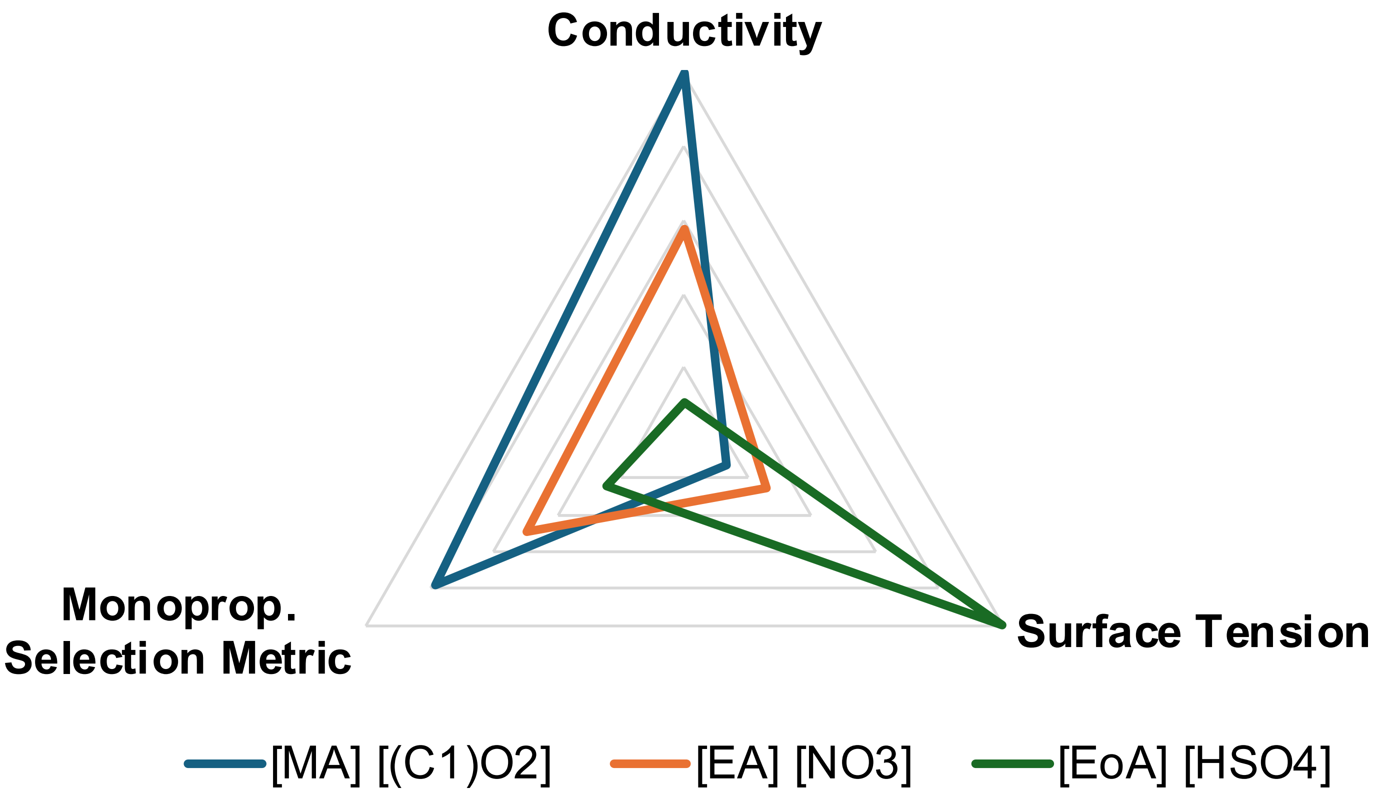

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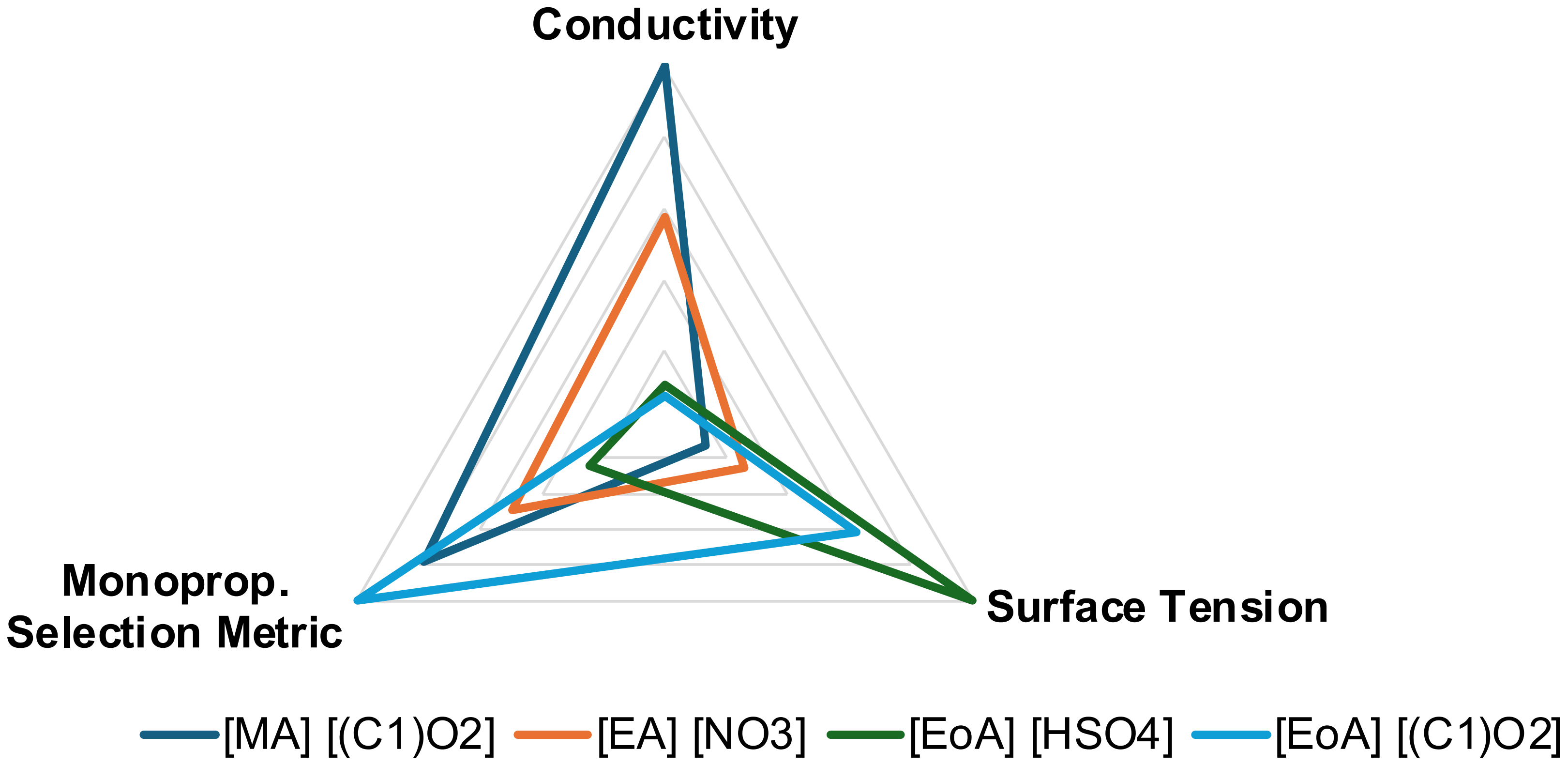
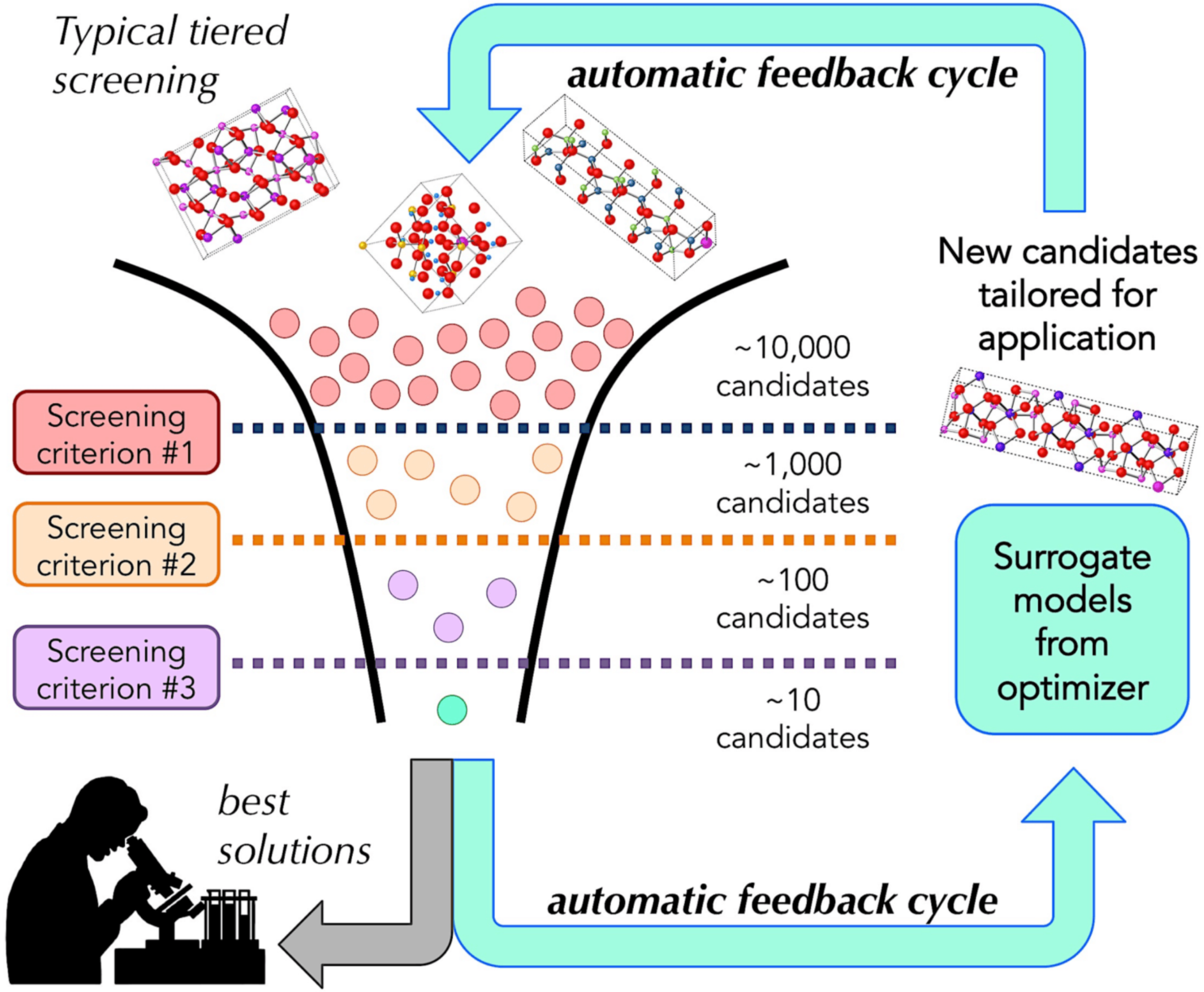
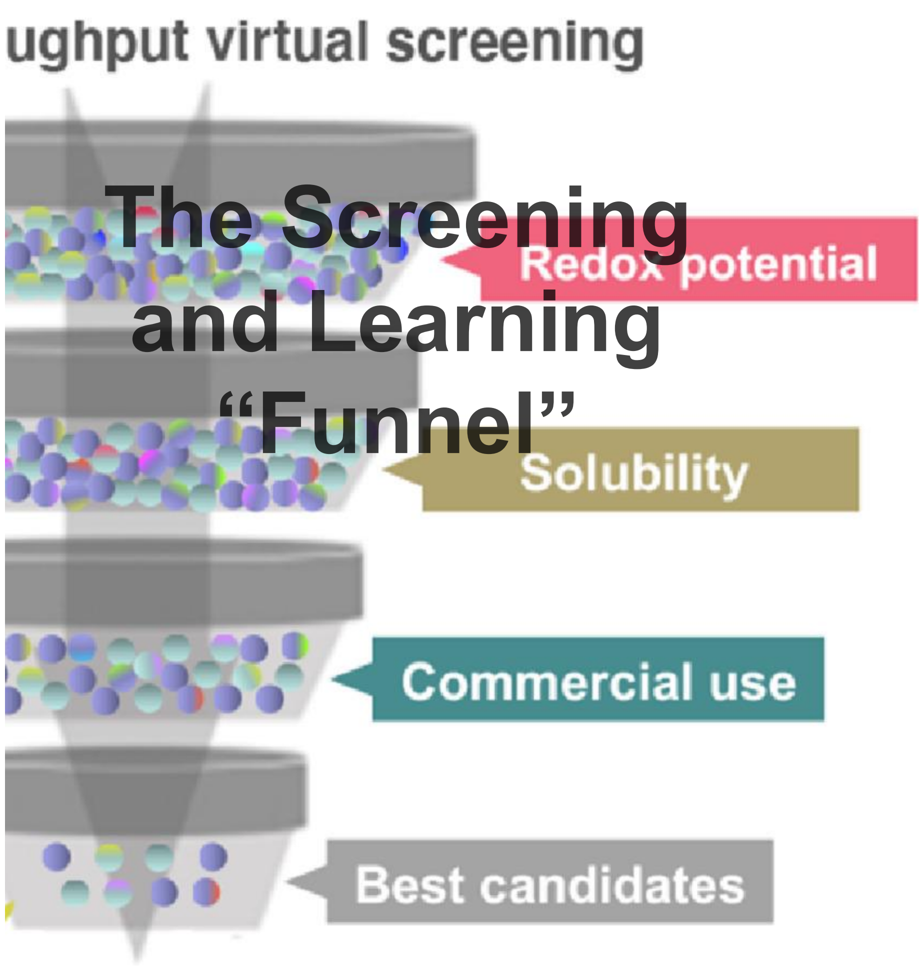


Ewan Fonda-Marsland and Charlie Ryan. "Preliminary Ionic Liquid Propellant Selection for Dual-Mode Micro-Propulsion Systems," AIAA 2017-5019. *53rd AIAA/SAE/ASEE Joint Propulsion Conference*. July 2017.

High-throughput Screening





The Screening and Learning "Funnel"

https:
throu

https://www.mongodb.com/solutions/customer-case-studies/berkeley-lab

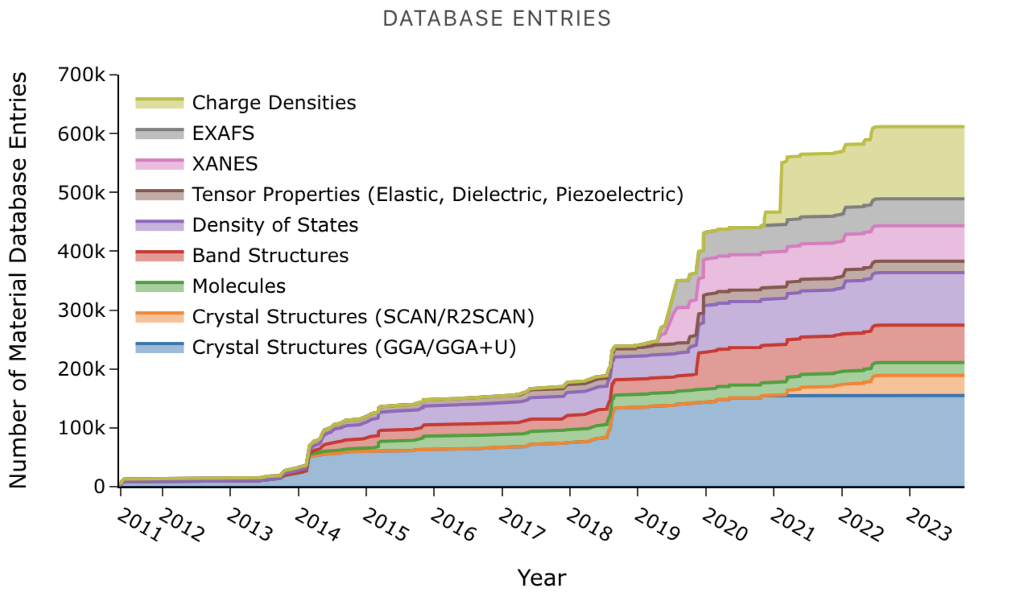
discovery of small electroactive molecules for energy
w batteries. *Energy Storage Materials,* 47, **2022**, 167-177.

The Materials Project

Prof. Kristin A. Persson

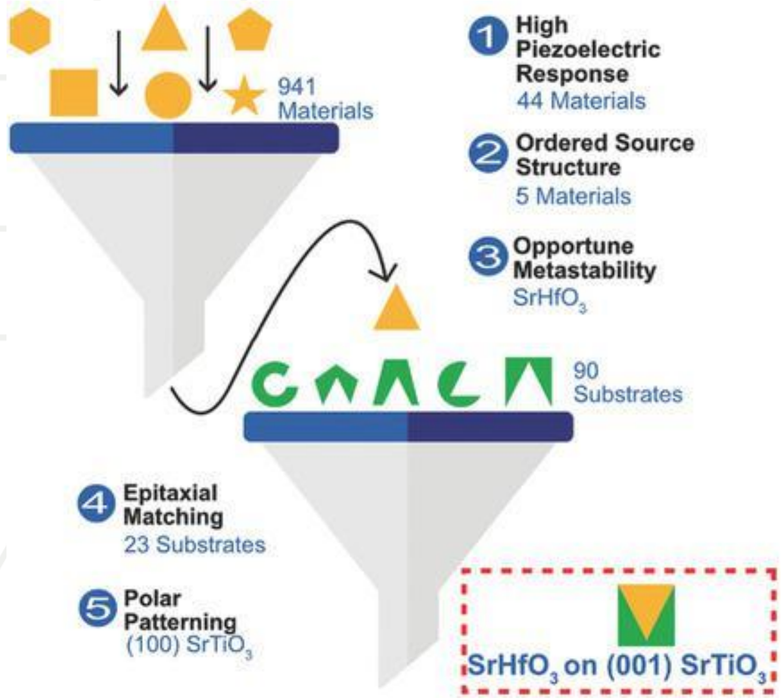
The Materials Project by the numbers

MATERIALS	REGISTERED USERS
154,718	460,000+
INTERCALATION ELECTRODES	**CITATIONS**
4,351	42,000+
MOLECULES	**CPU HOURS/YEAR**
172,874	100 million



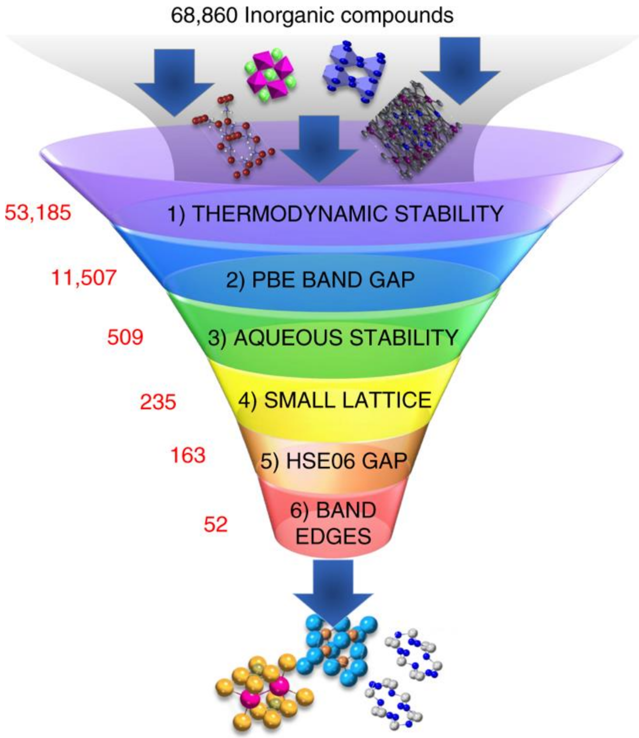
"Harnessing the power of **supercomputing** and state-of-the-art methods, the Materials Project provides open web-based access to computed information on known and predicted materials as well as powerful analysis tools **to inspire and design novel materials**."

The Materials Project has led to the discovery of…



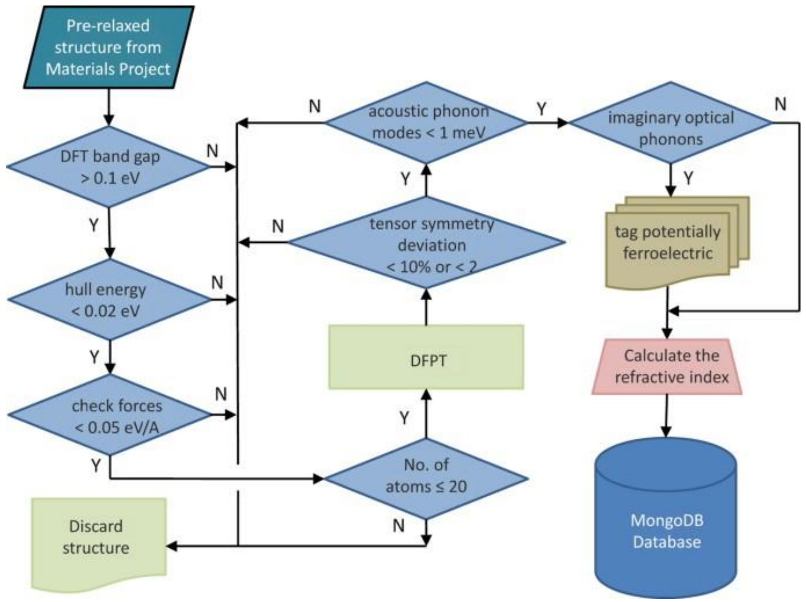
L. M. Garten, S. Dwaraknath, J. Walker, J. S. Mangum, P. F. Ndione, Y. Park, D. A. Beaton, V. Gopalan, B. P. Gorman, L. T. Schelhas, M. F. Toney, S. Trolier-McKinstry, K. A. Persson, D. S. Ginley, *Adv. Mater.* 2018, 30, 1800559.

piezoelectric materials



Singh, A.K., Montoya, J.H., Gregoire, J.M. *et al.* Robust and synthesizable photocatalysts for CO_2 reduction: a data-driven materials discovery. *Nat Commun* **10**, 443 (2019).

photocatalysts



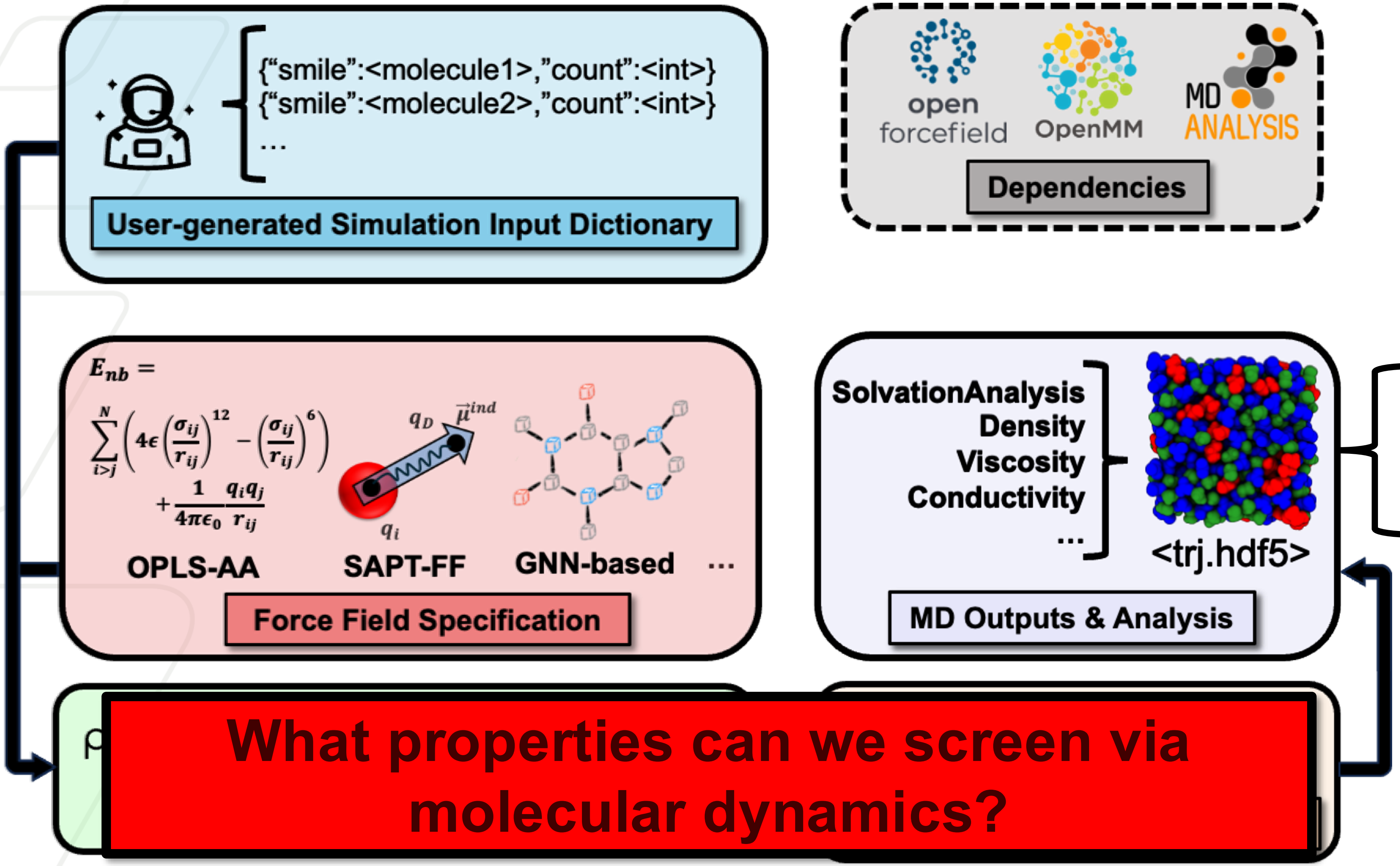
Petousis, I., Mrdjenovich, D., Ballouz, E. *et al.* High-throughput screening of inorganic compounds for the discovery of novel dielectric and optical materials. *Sci Data* **4**, 160134 (2017).

dielectrics

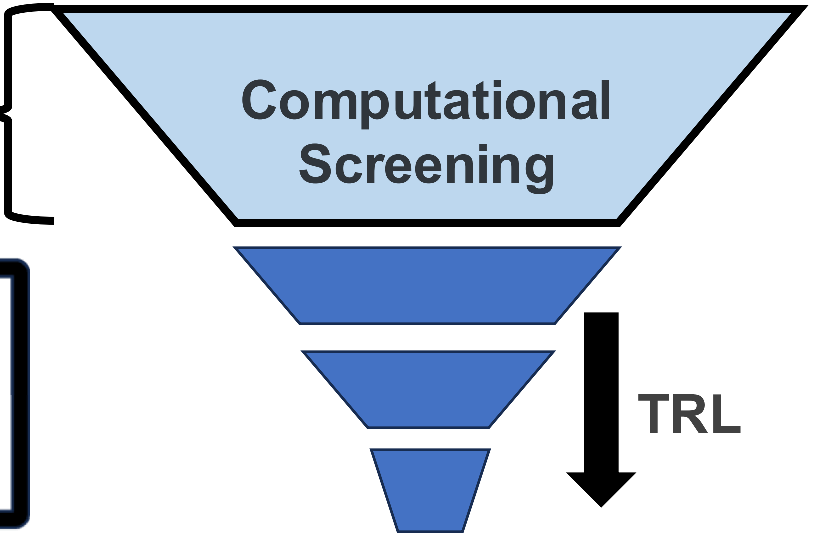
- **Objective 1**: Increase selection space of multimode propulsion propellants
  - **Approach**: computational, high-throughput screening

- **Objective 2**: Develop a database of computed ionic liquids properties
  - **Approach**: molecular dynamics

Computational High-throughput Screening for Ionic Liquids



Orion Cohen



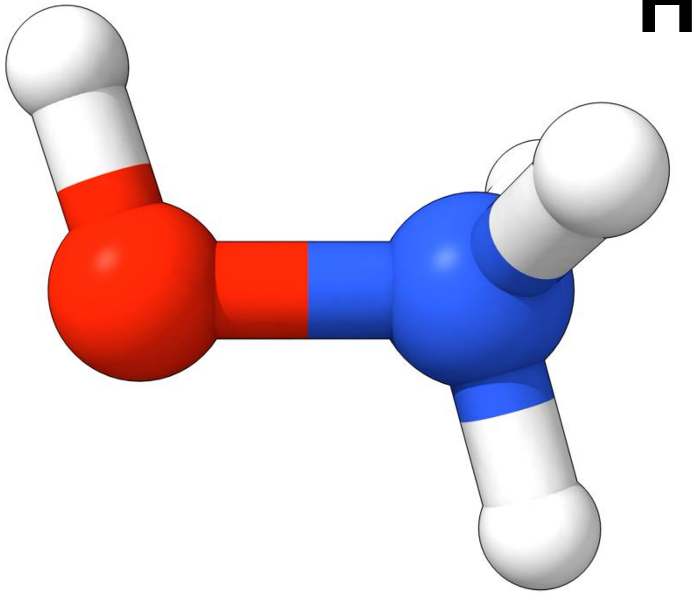
Computing propellant properties via MD

Case Study: HAN and HEHN

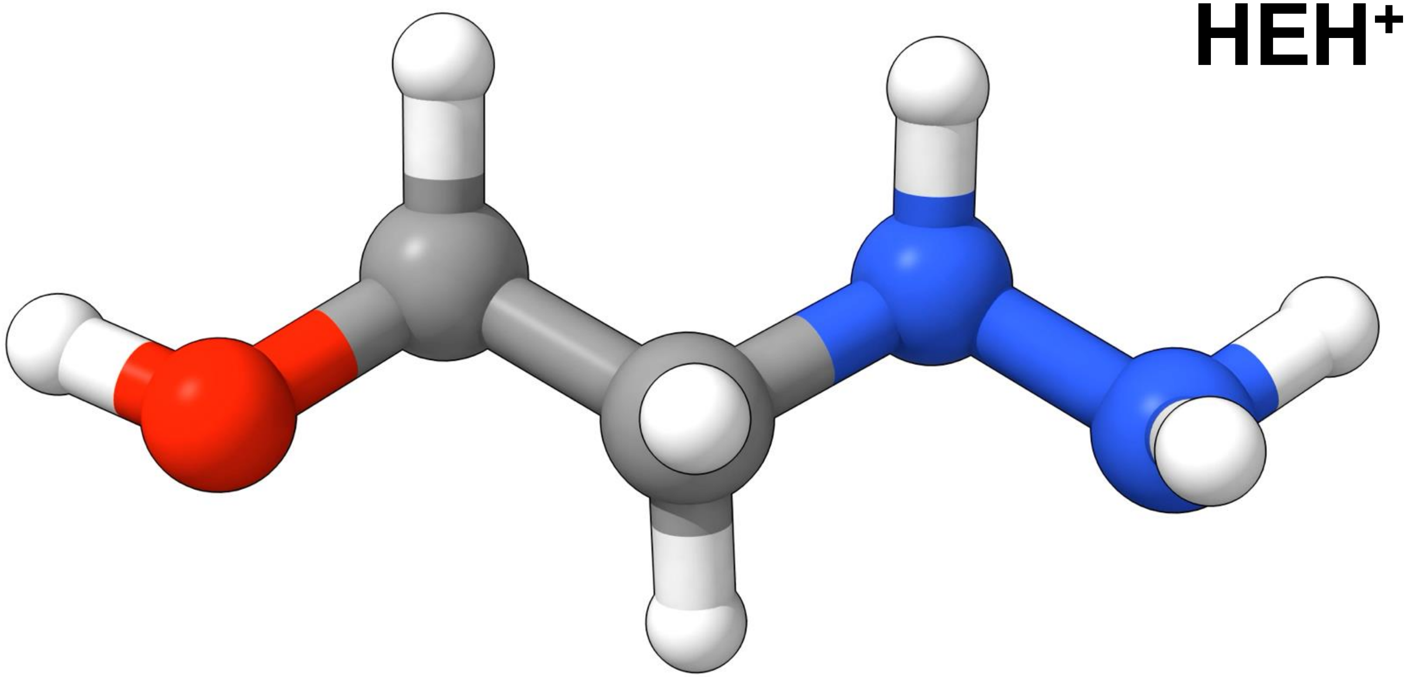
Shehan M. Parmar, Daniel D. Depew, Richard E. Wirz, and Ghanshyam L. Vaghjiani,
"Structural Properties of HEHN- and HAN-Based Ionic Liquid Mixtures: A Polarizable Molecular Dynamics Study,"
The Journal of Physical Chemistry B **2023** *127* (40), 8616-8633

HAN and HEHN

HA+



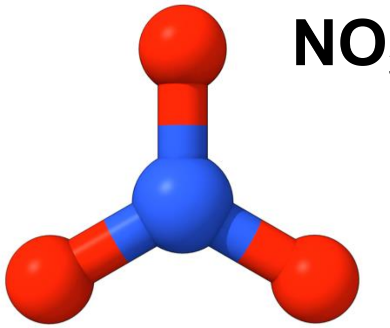
HEH+

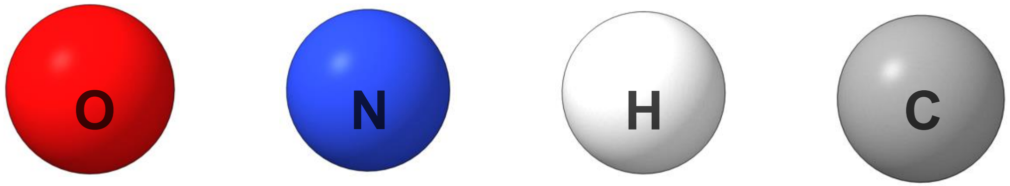


~2-3 Å

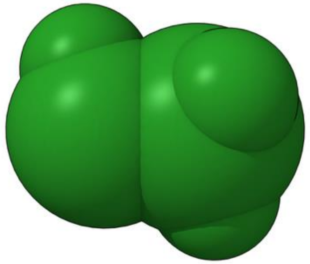
~6-7 Å

NO_3^-

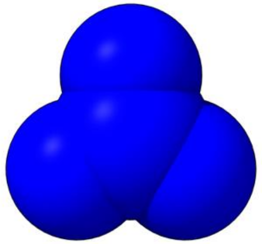




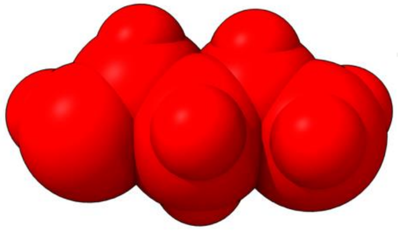
Simulation Domains



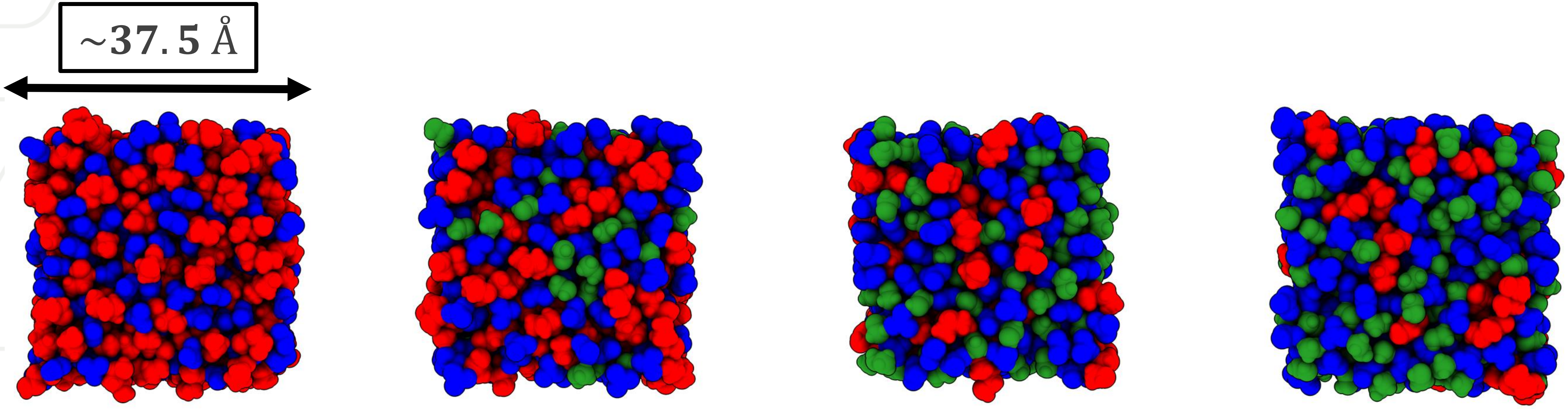
HA^+



NO_3^-



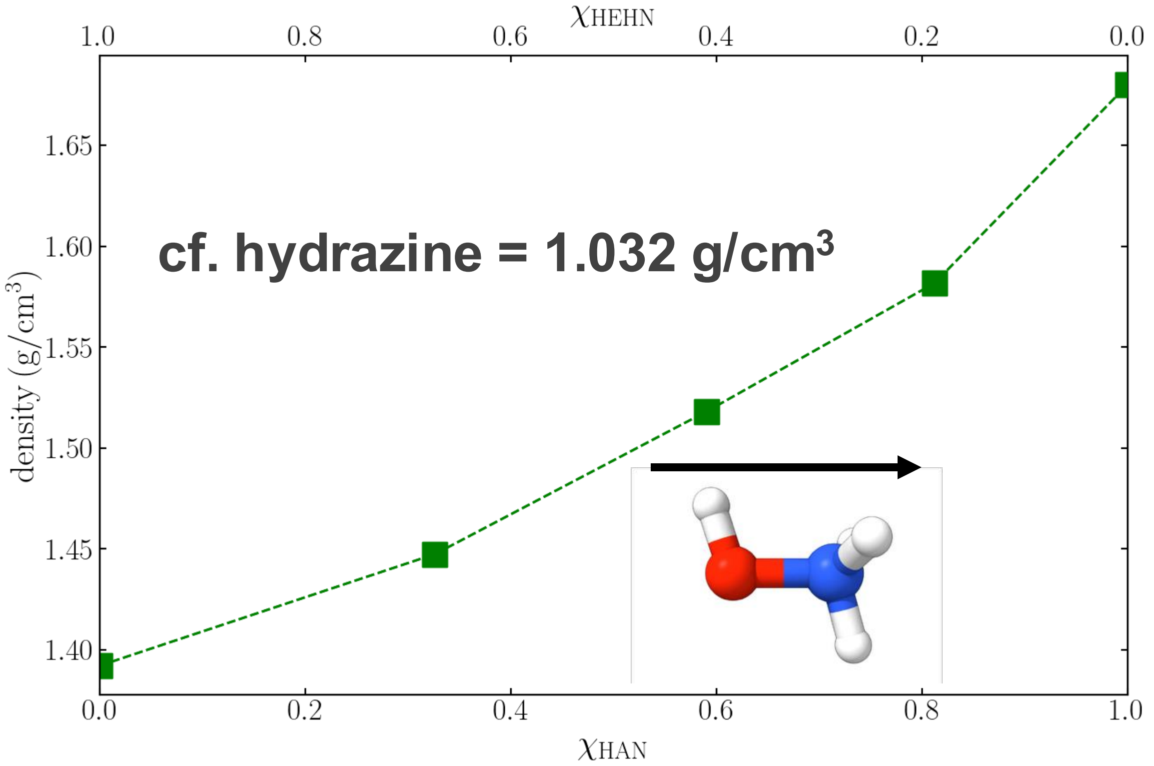
HEH^+



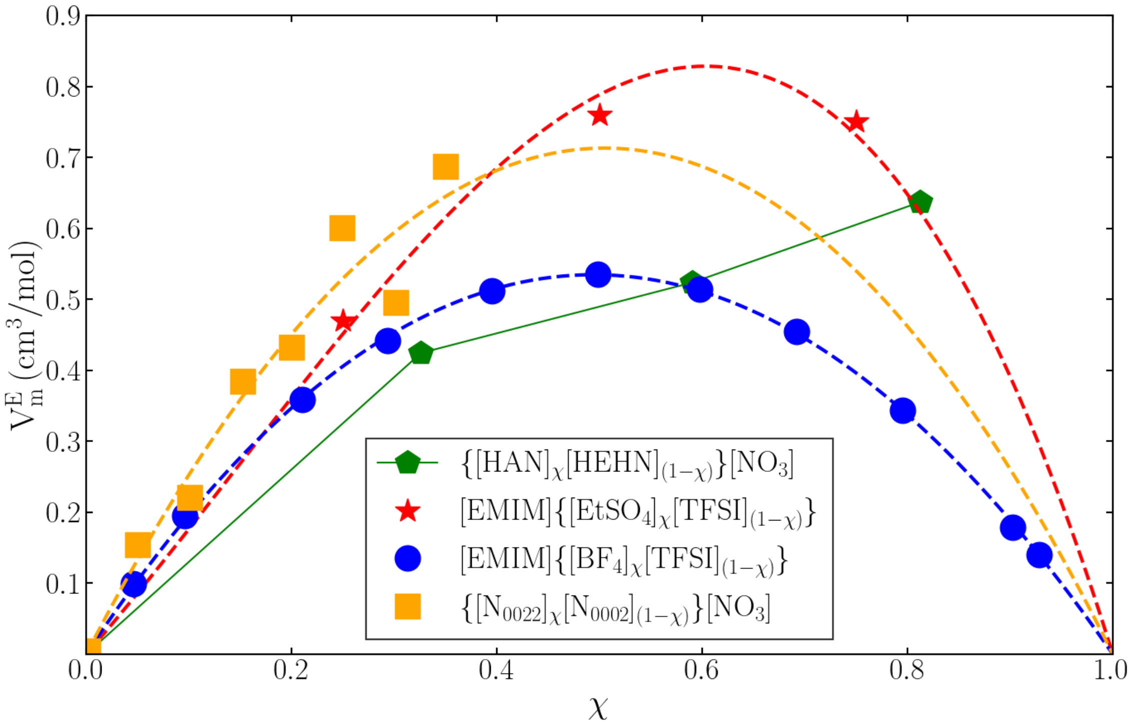
$\chi_{HAN} = 0.0$ $\chi_{HAN} = 0.326$ $\chi_{HAN} = 0.591$ $\chi_{HAN} = 0.812$

Shehan M. Parmar, Daniel D. Depew, Richard E. Wirz, and Ghanshyam L. Vaghjiani. *The Journal of Physical Chemistry B* **2023** *127* (40), 8616-8633

Density and Excess Molar Volume

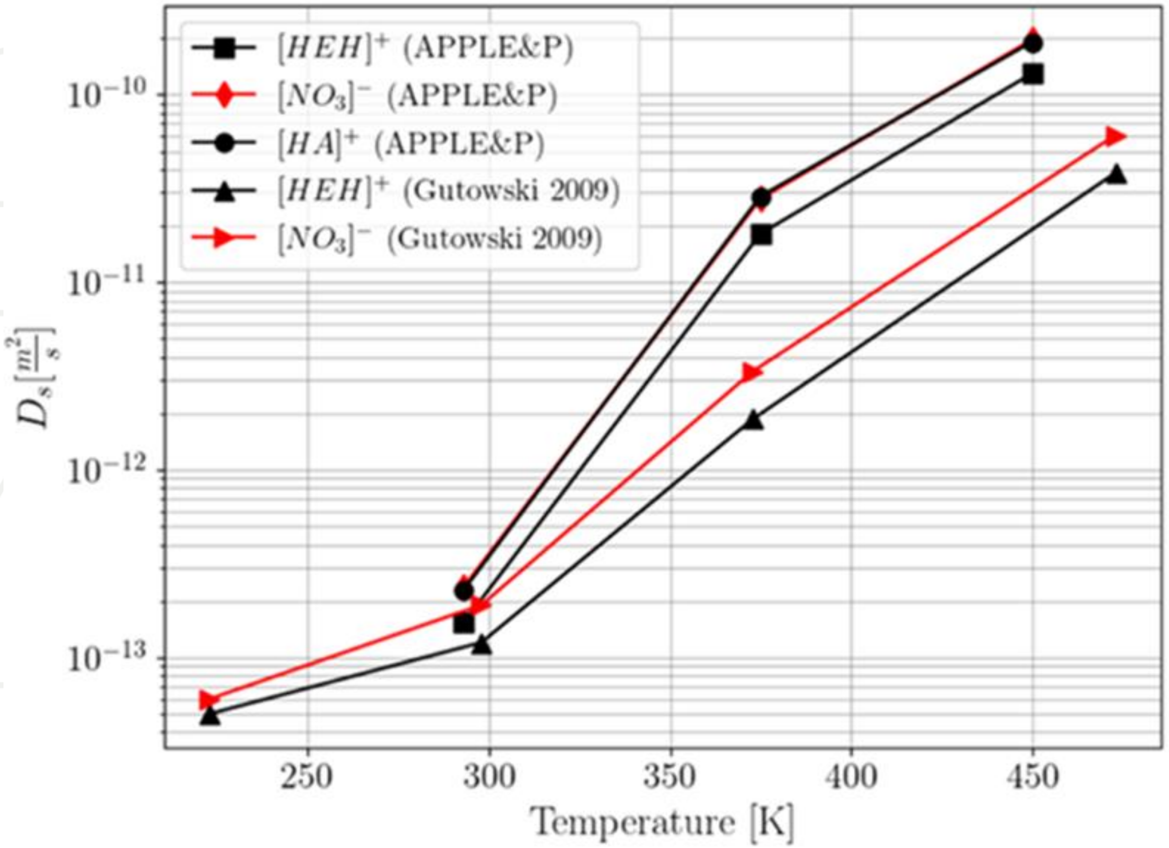


$$V_M^E = V_{mixture} - V_{HAN} - V_{HEHN}$$



Relatively high-magnitude excess molar volumes suggest partial immiscibility due to differences in cation sizes.

Transport Properties



<u>*Self-diffusion Coefficient*</u>:

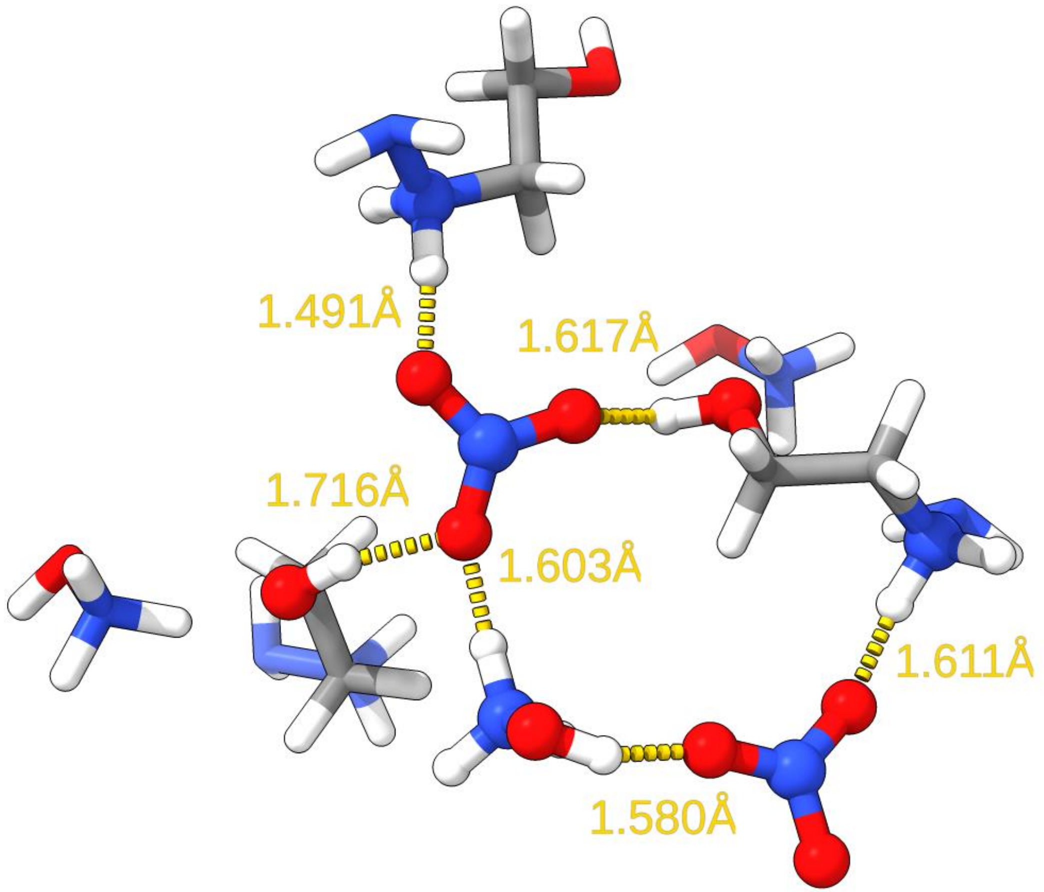
$$D_s = \frac{1}{6} lim_{t\to\infty} \frac{d}{dt} \langle |\bar{r}(t) - \bar{r}(0)|^2 \rangle$$

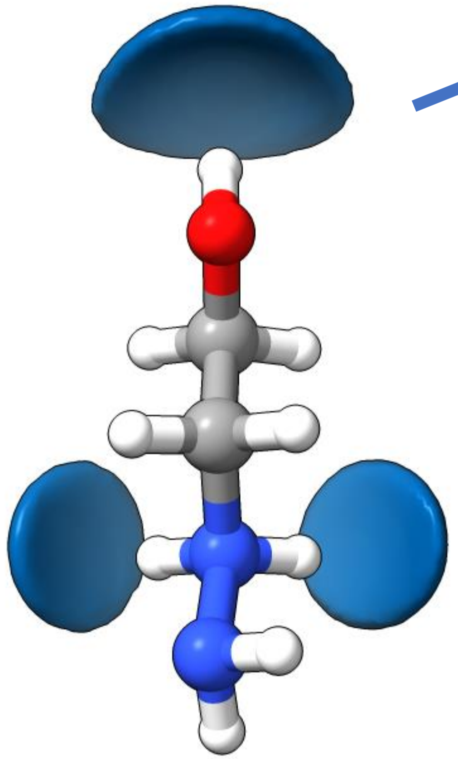
<u>*Viscosity*</u>:

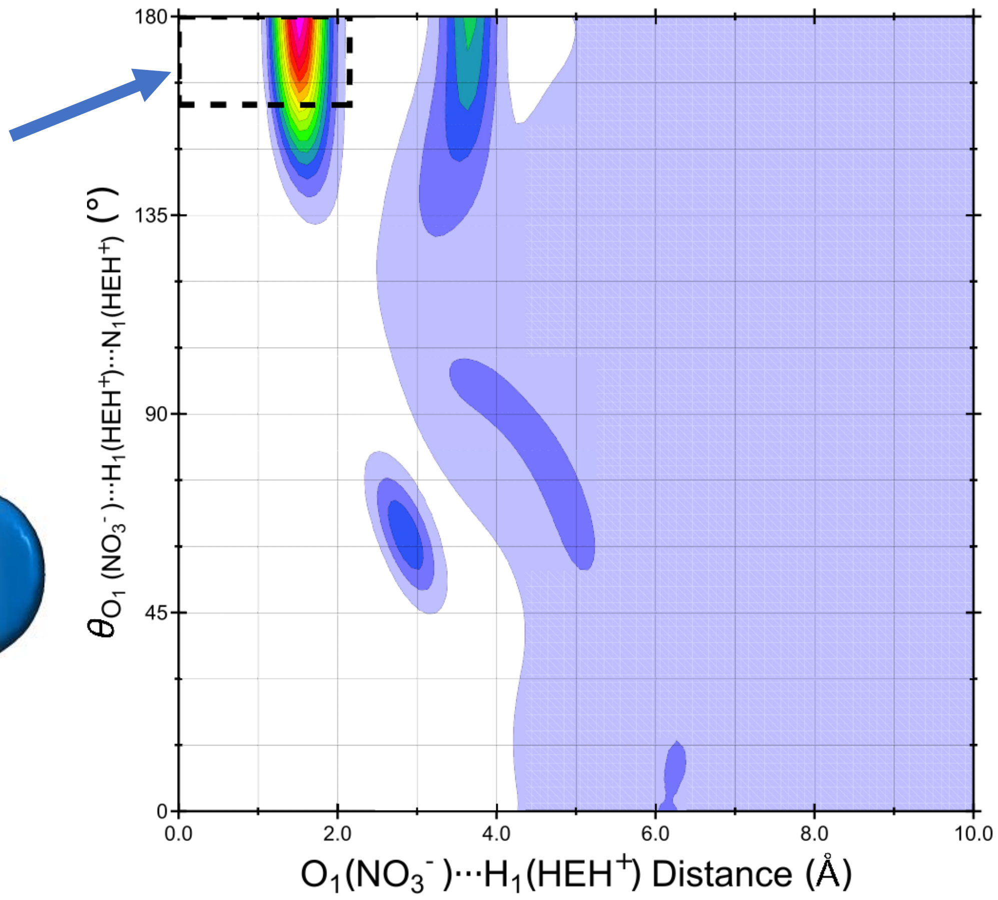
$$\eta \propto \frac{T}{D_s}$$

Self-diffusion coefficients indicate slow ion dynamics linked to high viscosities.

Hydrogen Bonding, a “coordinate along proton transfer”



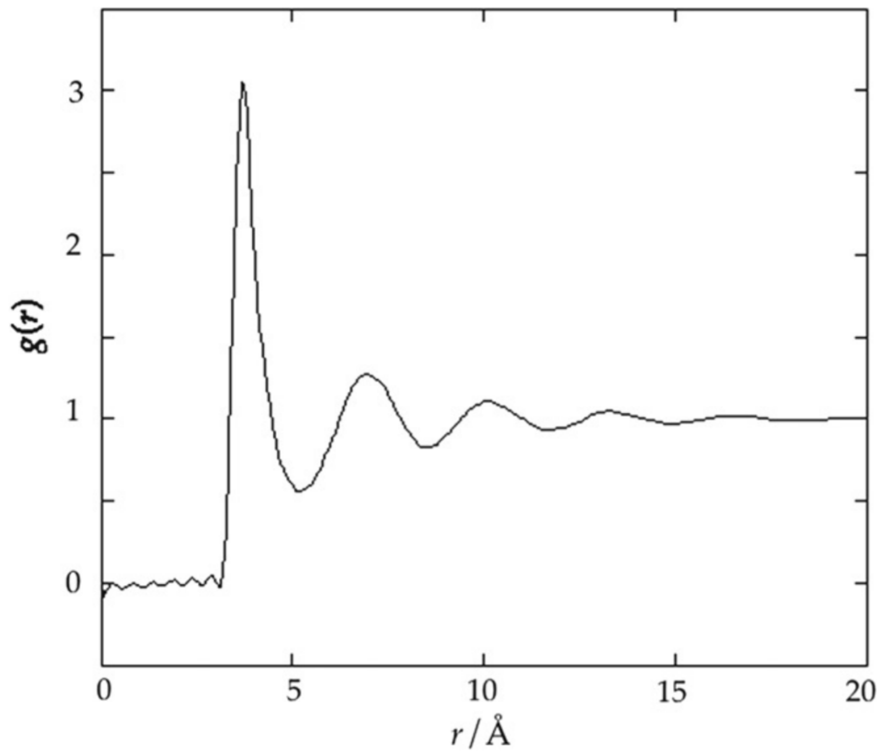




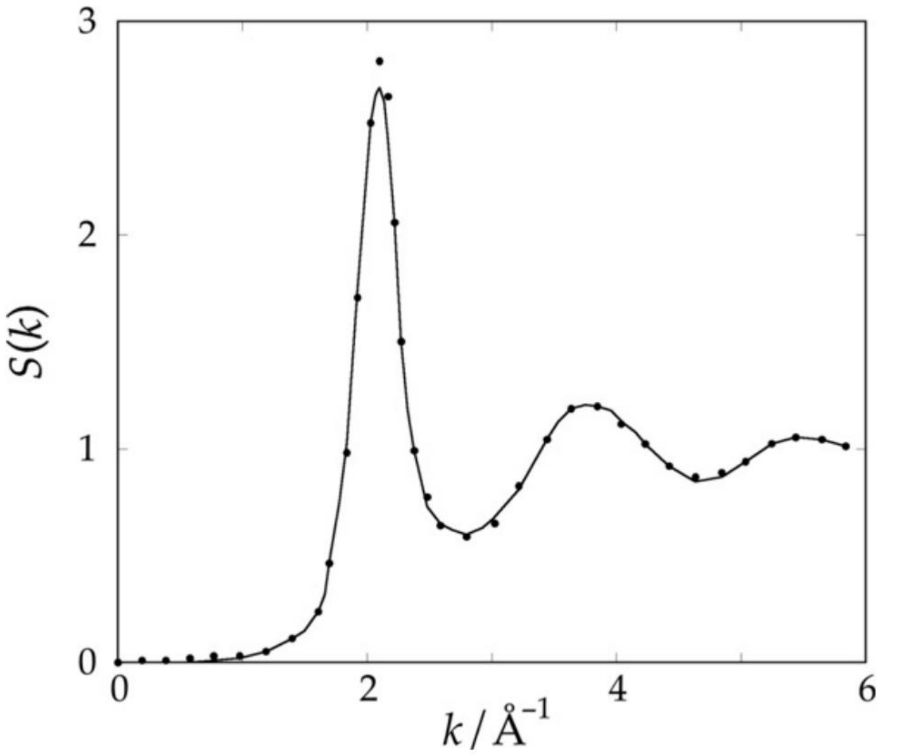
Hydrogen bond dominate local structure and can be unambiguously classified based on strength and linearity.

Miscibility with Water

Radial Distribution Function & Scattering Structure Factor



FFT



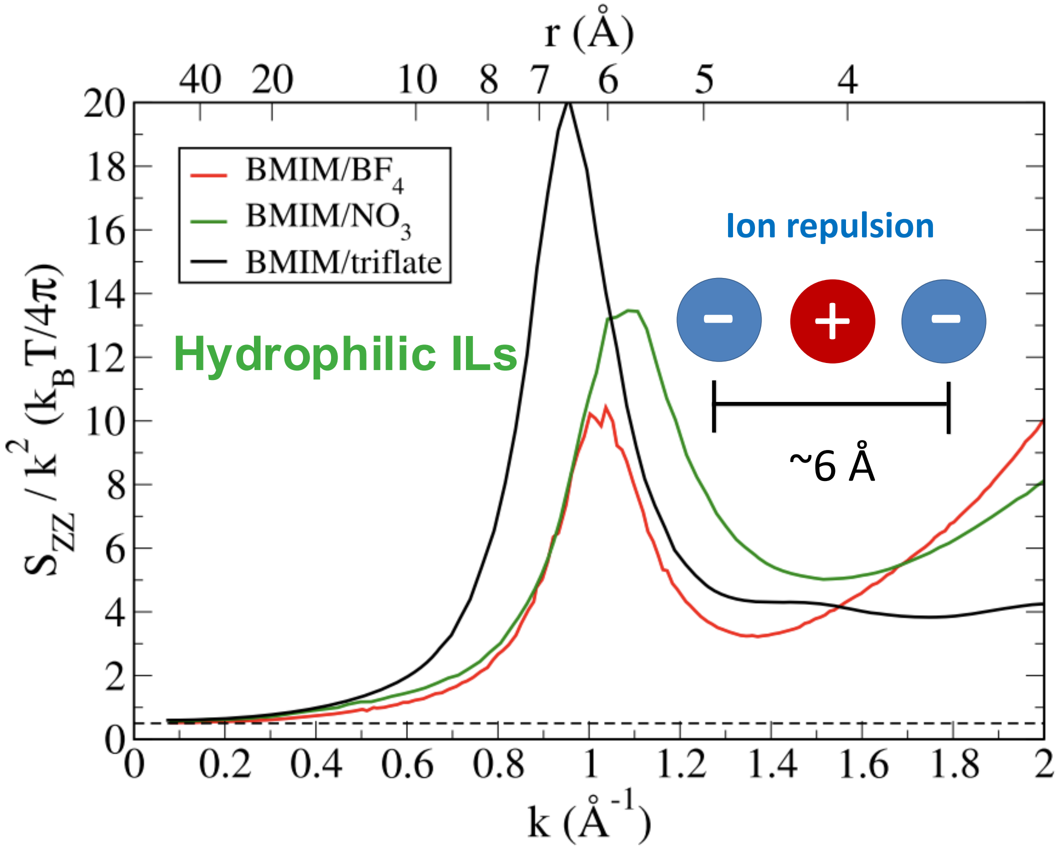
Real space

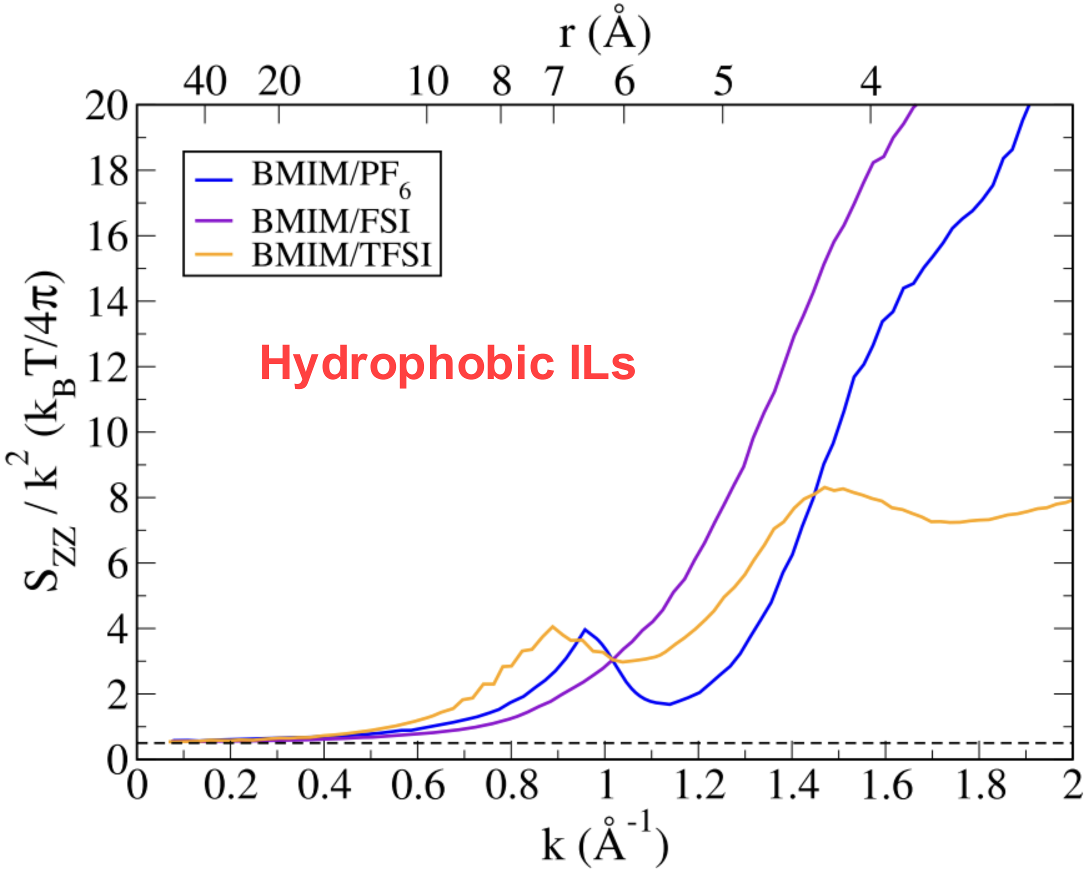
Reciprocal space

Radial distribution functions (RDFs), g(r), and the scattering structure factors, S(k), characterize key atomic length scales.

IL/Water Miscibility via Electrostatics

Prof. Jesse McDaniel





Jesse G. McDaniel and Archana Verma. *The Journal of Physical Chemistry B* **2019** *123* (25), 5343-5356

The charge correlation structure factor unambiguously classifies IL miscibility with water.

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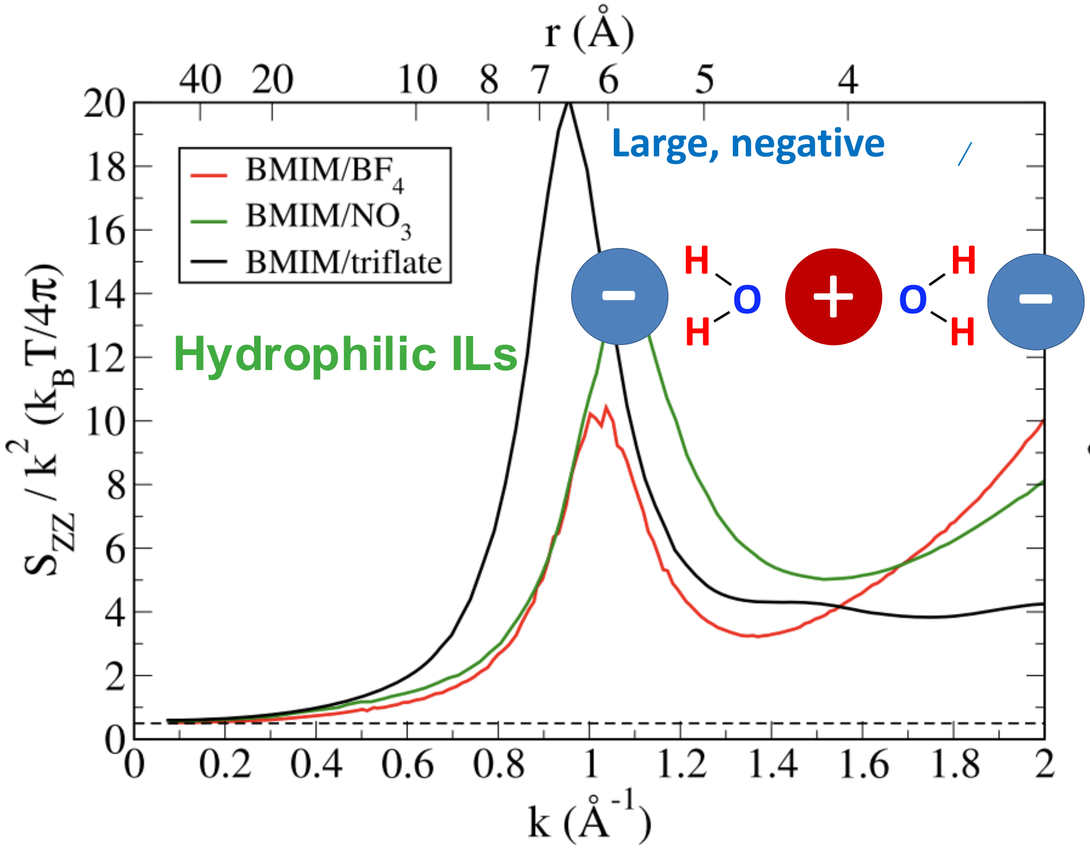

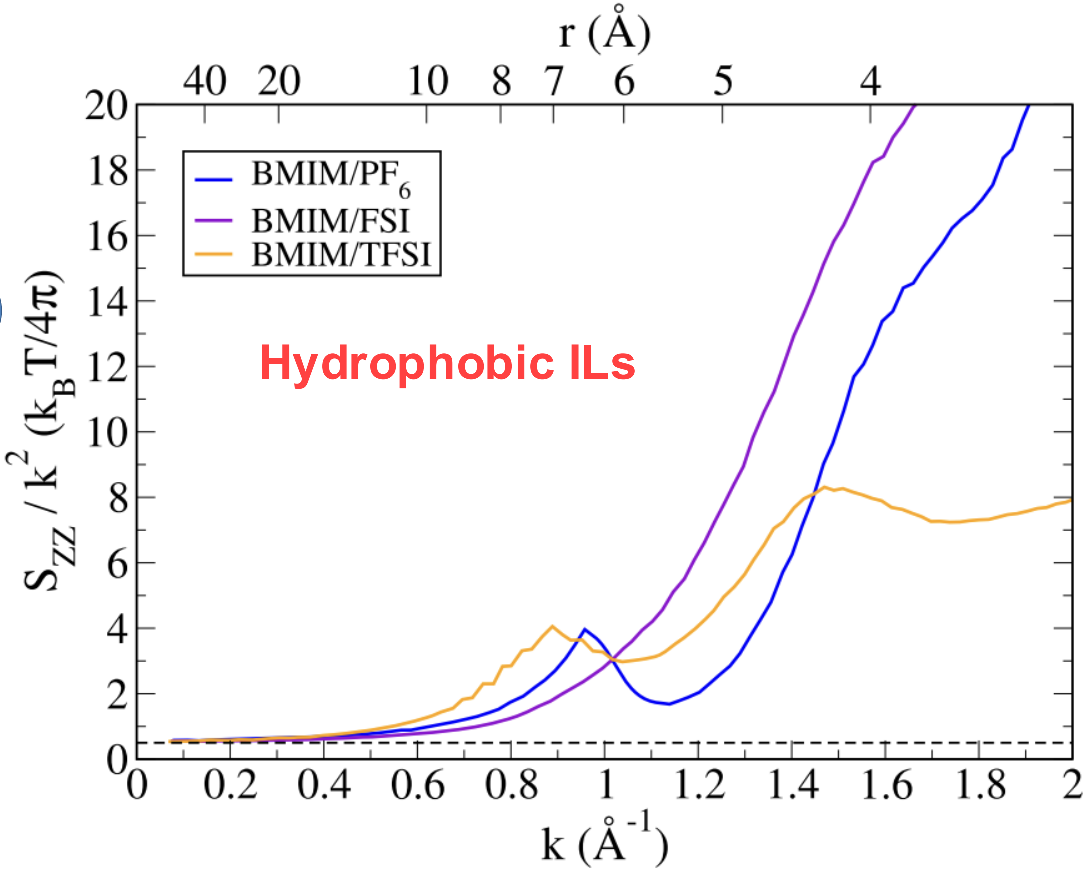

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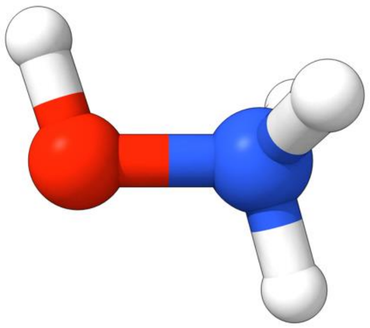
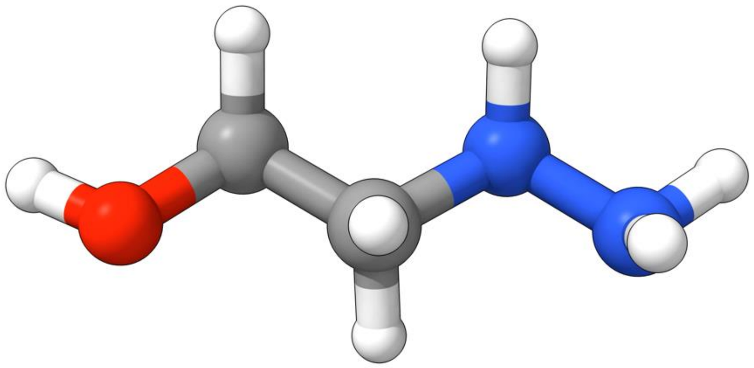
Conclusions



- A deployable computational, high-throughput screening workflow can be attractive for MMP
- Computational methods can provide screening, before experiments, of critical propellant propertie
  - ✓Pairwise distribution functions
  - ✓Density, excess molar volumes
  - ✓Miscibility w/ water
  - ✓Transport (conductivity, viscosity)



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