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The modern-day alchemist: using machine learning to design lubricants

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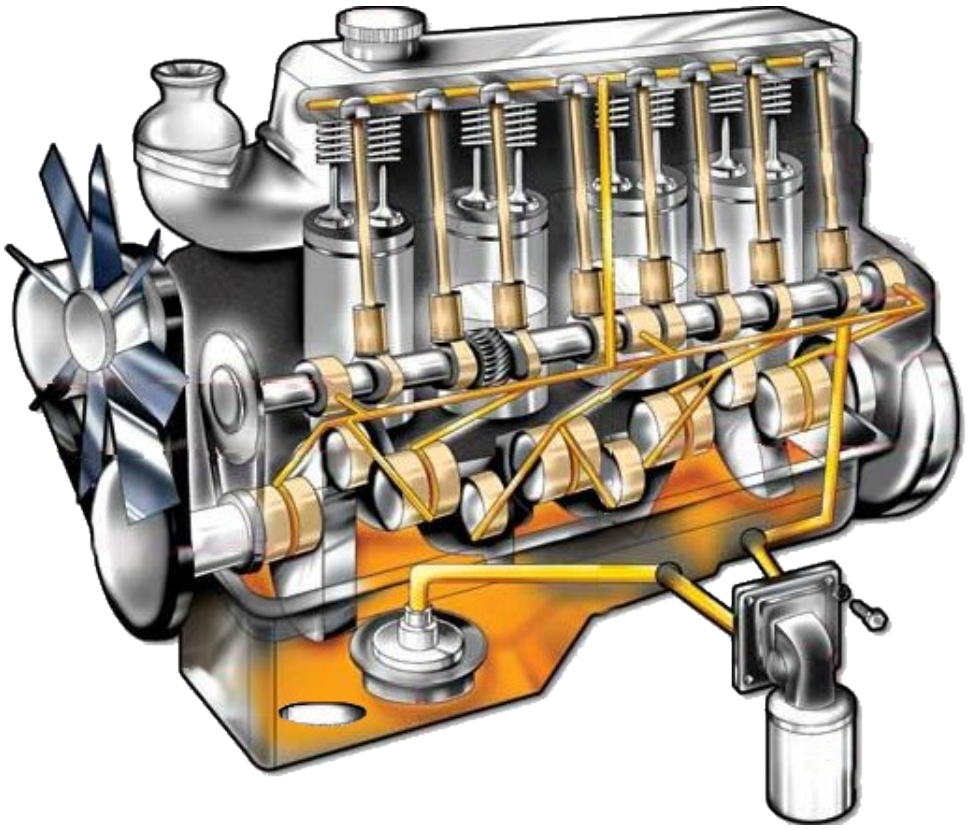
Les Bolton, Corneliu Buda, Phil Davies & Nikos Diamantonis

Theory of Condensed Matter group

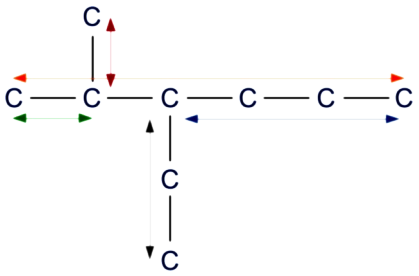
Purpose of lubricants



- Reduce friction between surfaces
- Protect surfaces from wear
- Liquid
- Transfer heat
- Remove dirt
- Prevent surface corrosion
- Not spontaneously combust

Neural network for lubricant design

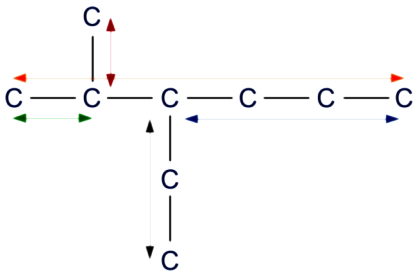
Structure



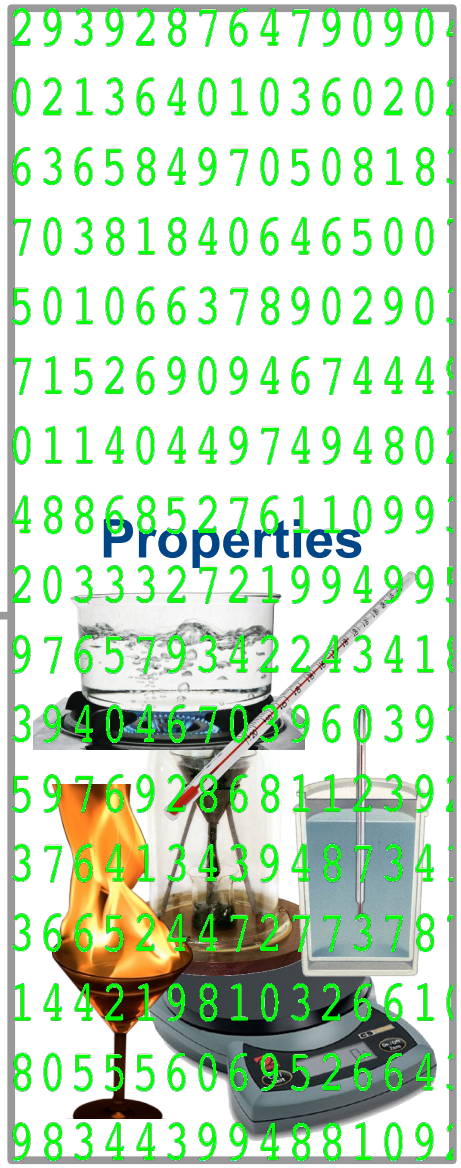
Properties

Train the neural network

Structure

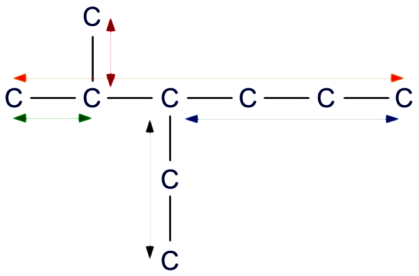


Properties



Predict using the neural network

Structure



Properties

Alchemite machine learning algorithm to

Train from sparse datasets

Merge simulations, physical laws, and experimental data

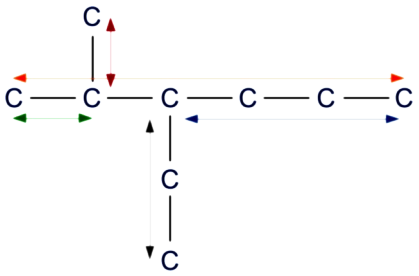
Reduce expensive and time consuming experiments

Generic with proven applications in materials discovery and drug design

Apply to linear and branched alkanes

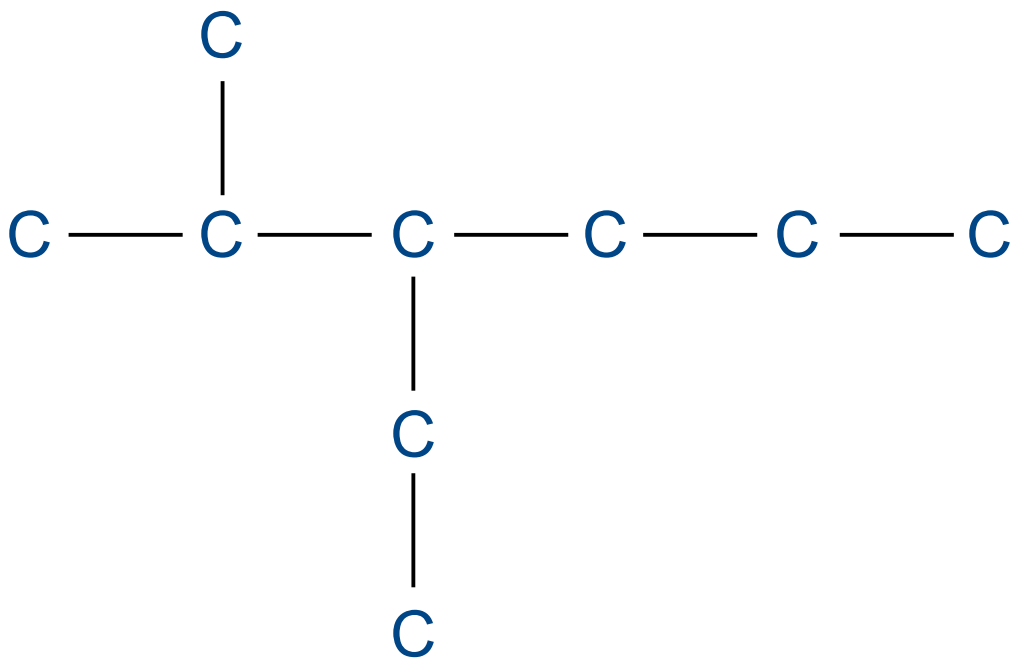
Predict using the neural network

Structure

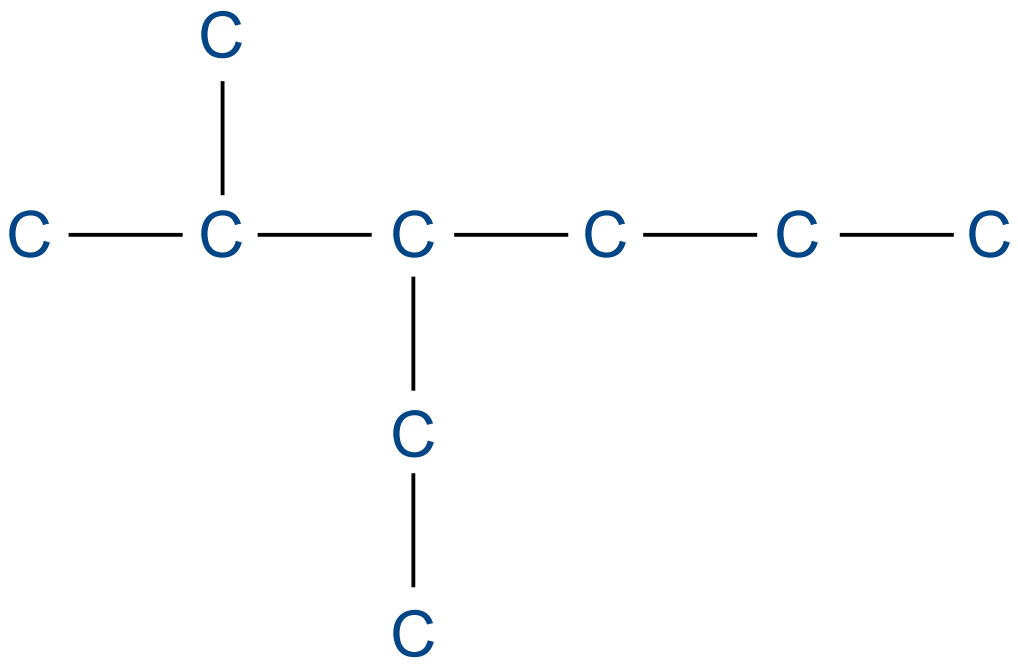


Properties

Typical lubricant hydrocarbon



Scope of lubricant study



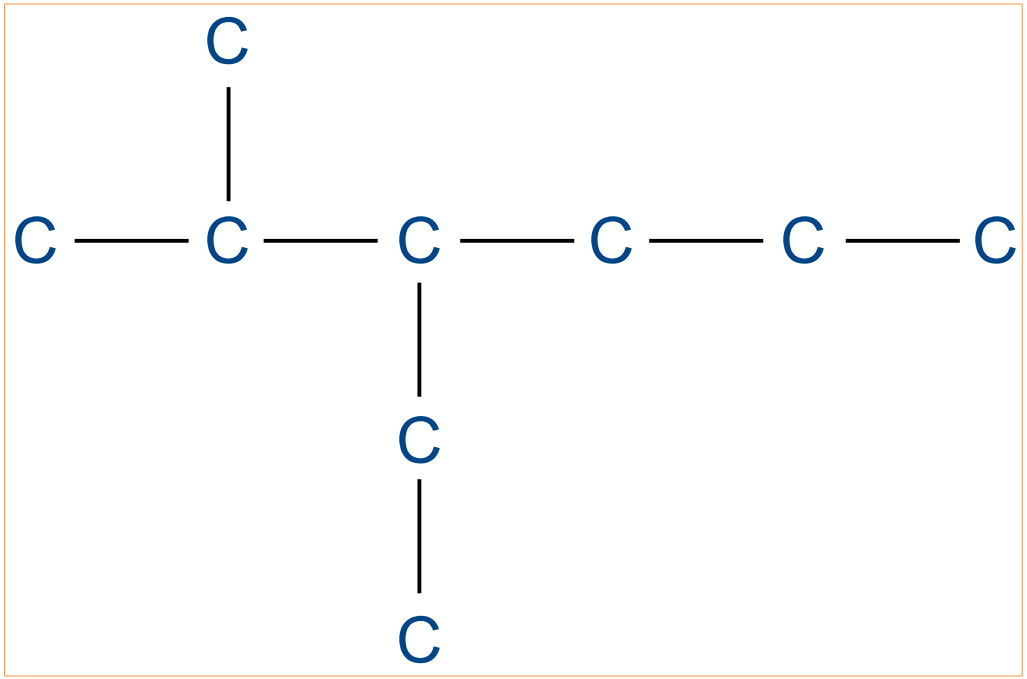
Comprise up to **thirty** carbon atoms

Consider up to **two** branches

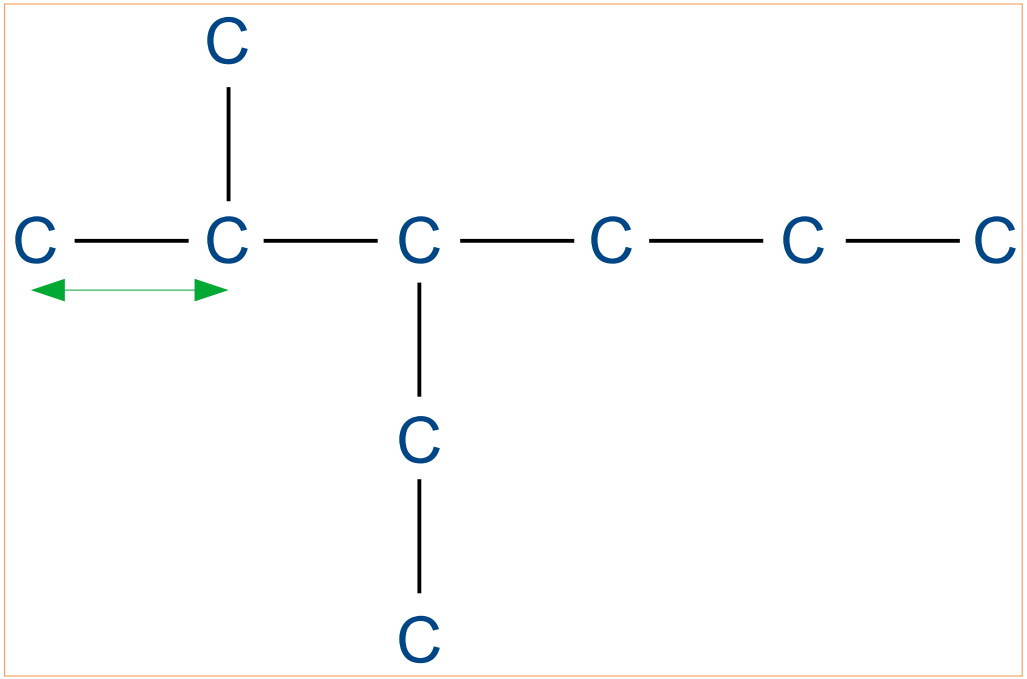
All **single** bonds, no additional elements

First component of basis set

Total number of C atoms



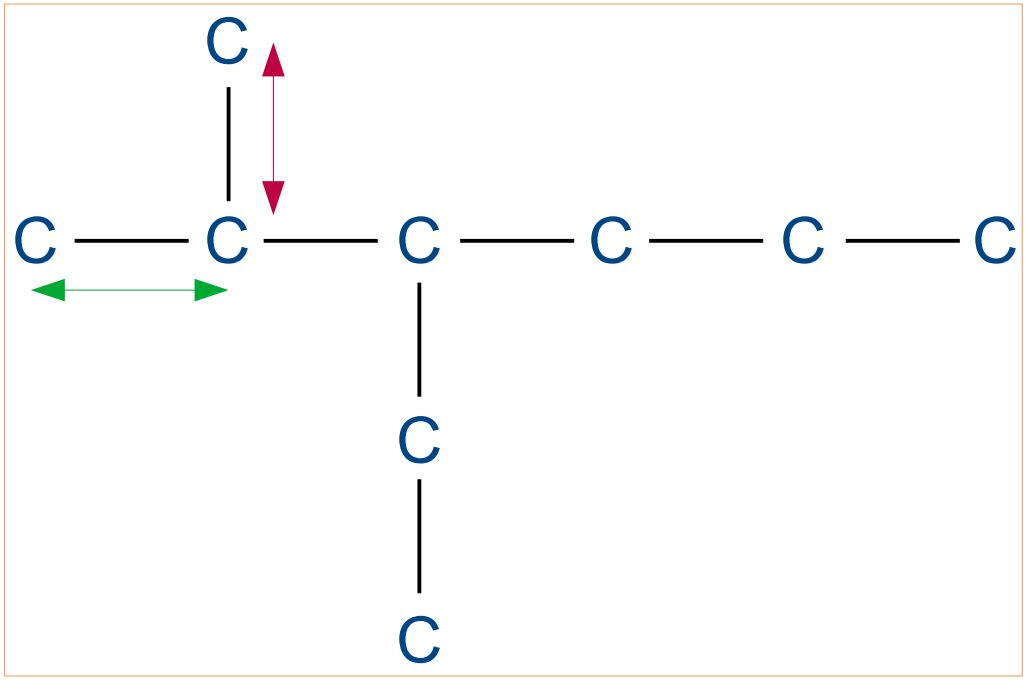
Second component of basis set



Total number of C atoms

Distance of first branch from end

Third component of basis set

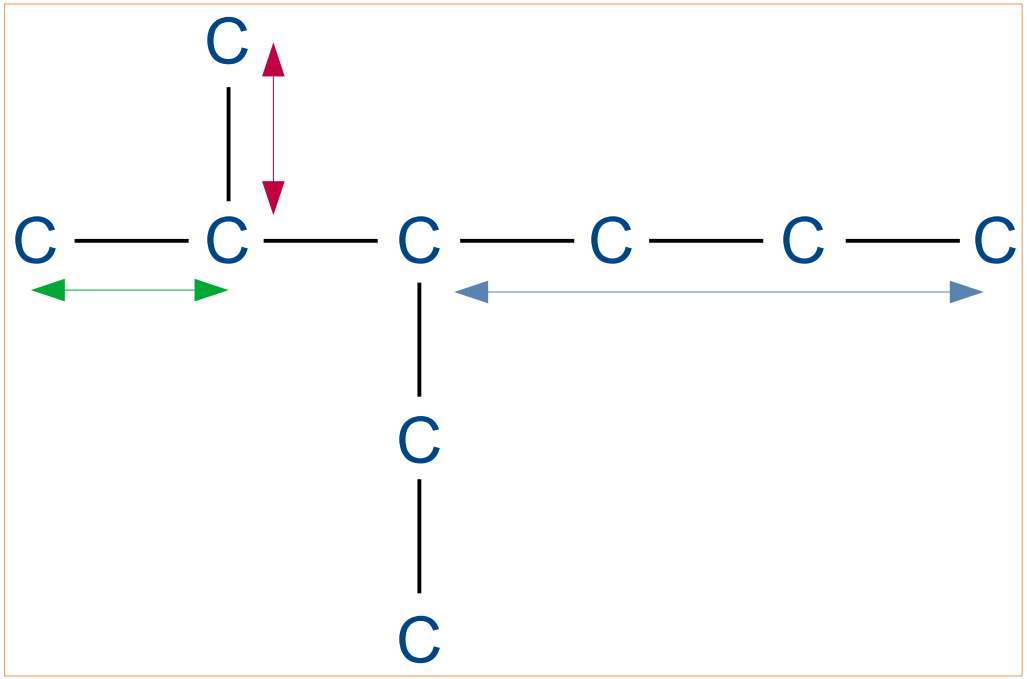


Total number of C atoms

Distance of first branch from end

Length of first branch

Fourth component of basis set



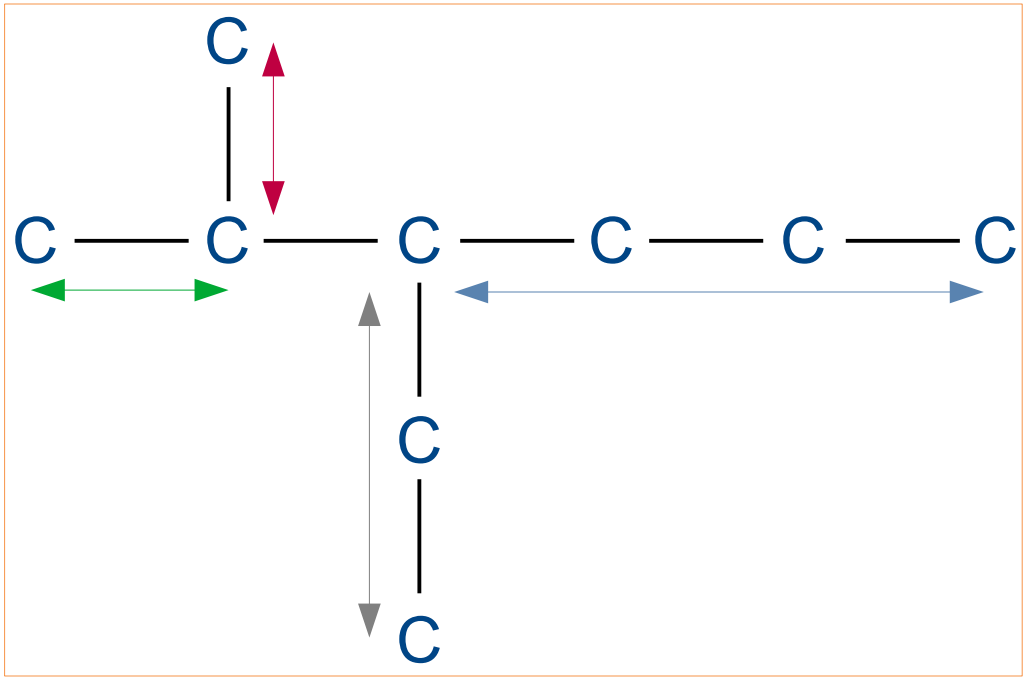
Total number of C atoms

Distance of first branch from end

Length of first branch

Distance of second branch from end

Fifth component of basis set



Total number of C atoms

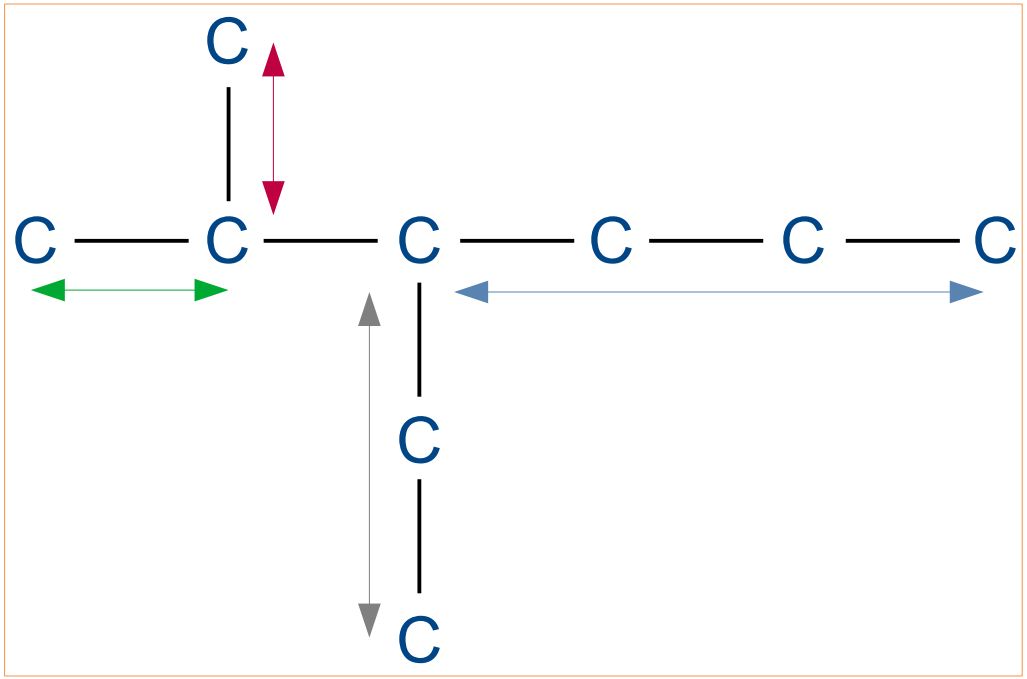
Distance of first branch from end

Length of first branch

Distance of second branch from end

Length of second branch

Full basis set



Total number of C atoms

Distance of first branch from end

Length of first branch

Distance of second branch from end

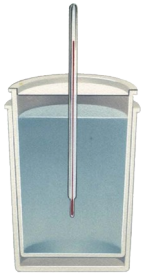
Length of second branch

(9,1,1,3,2)

Target properties

Melting point

Heat capacity



Boiling point

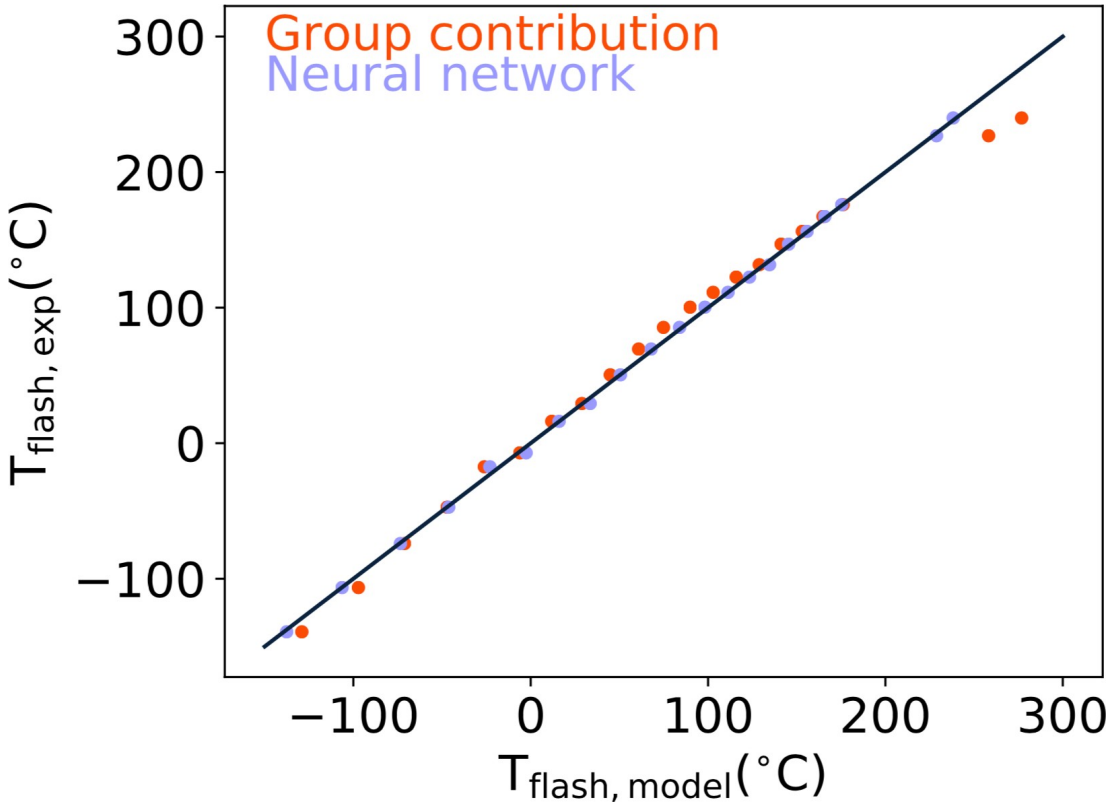
Vapor pressure

Density

Flash point

Viscosity index

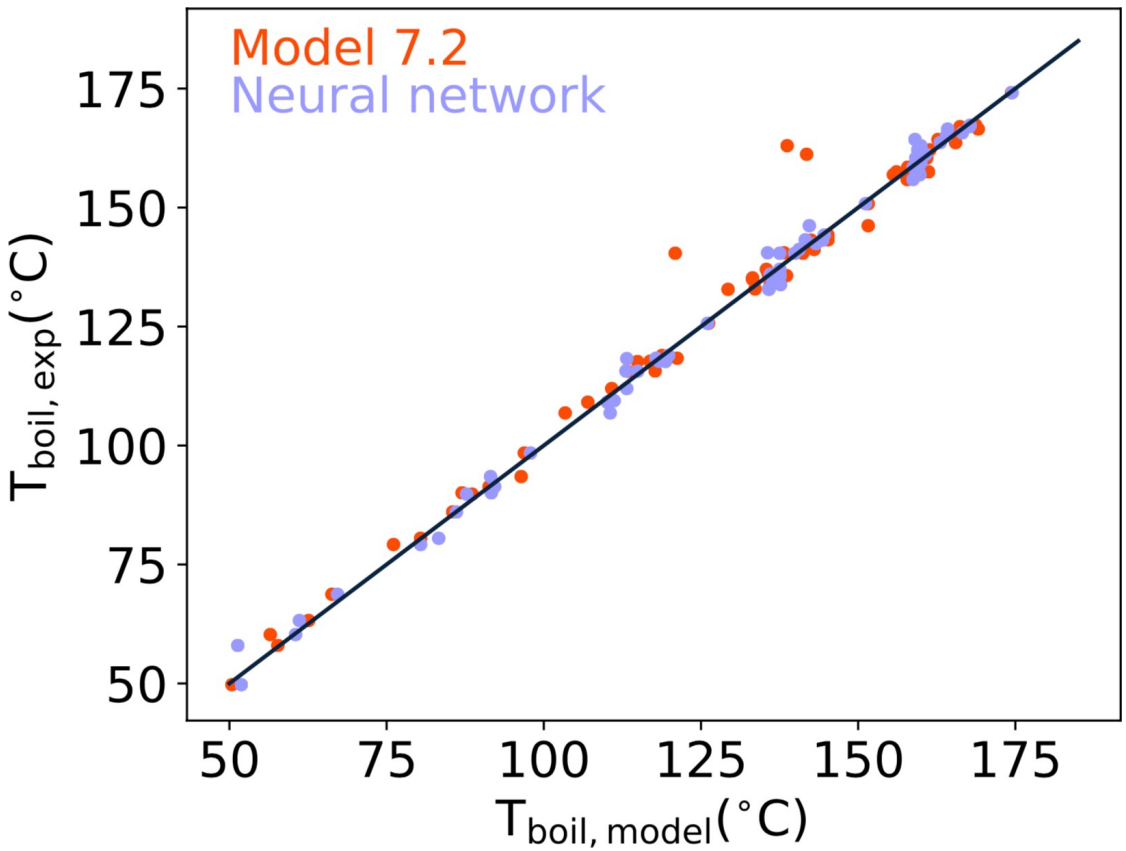
Flash point



Neural network R^2=0.997

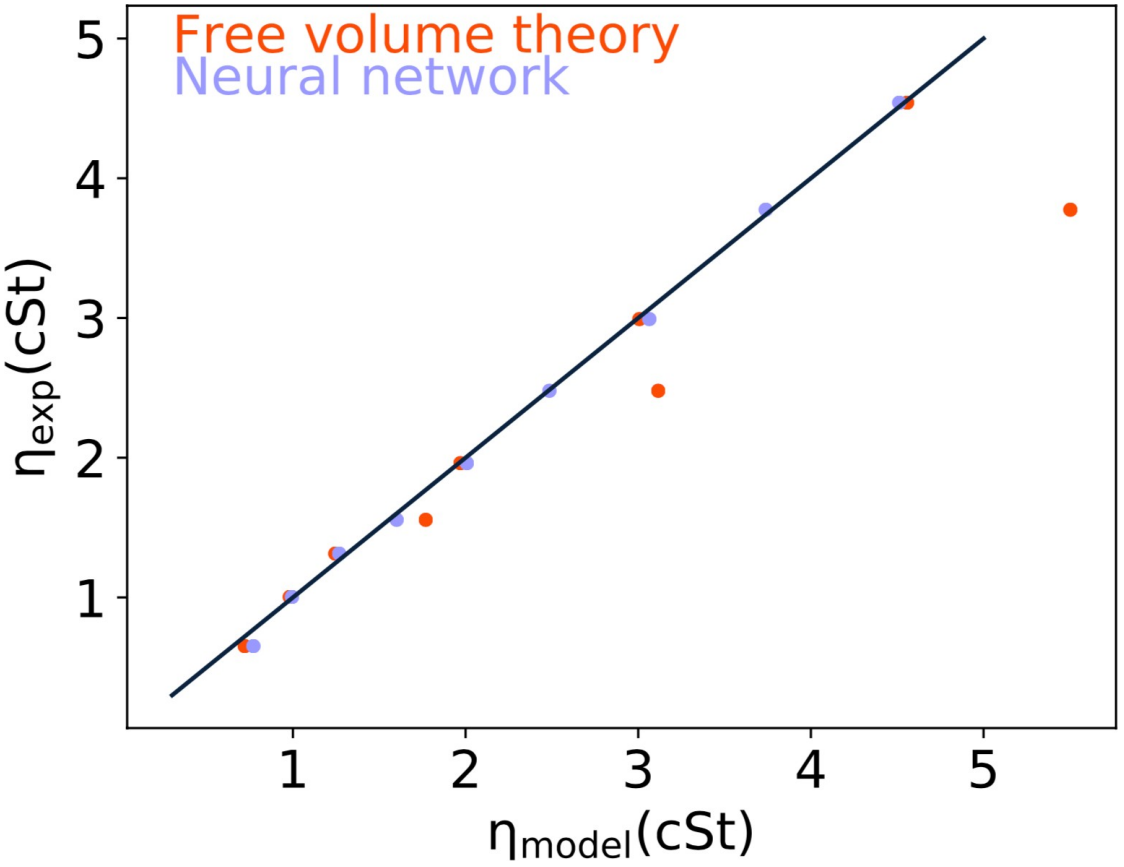
Group contribution R^2=0.971

Boiling point



Neural network	R^2=0.992
Model 7.2	R^2=0.977
Model 7.3	R^2=0.975

Kinematic viscosity



Neural network R^2=0.998

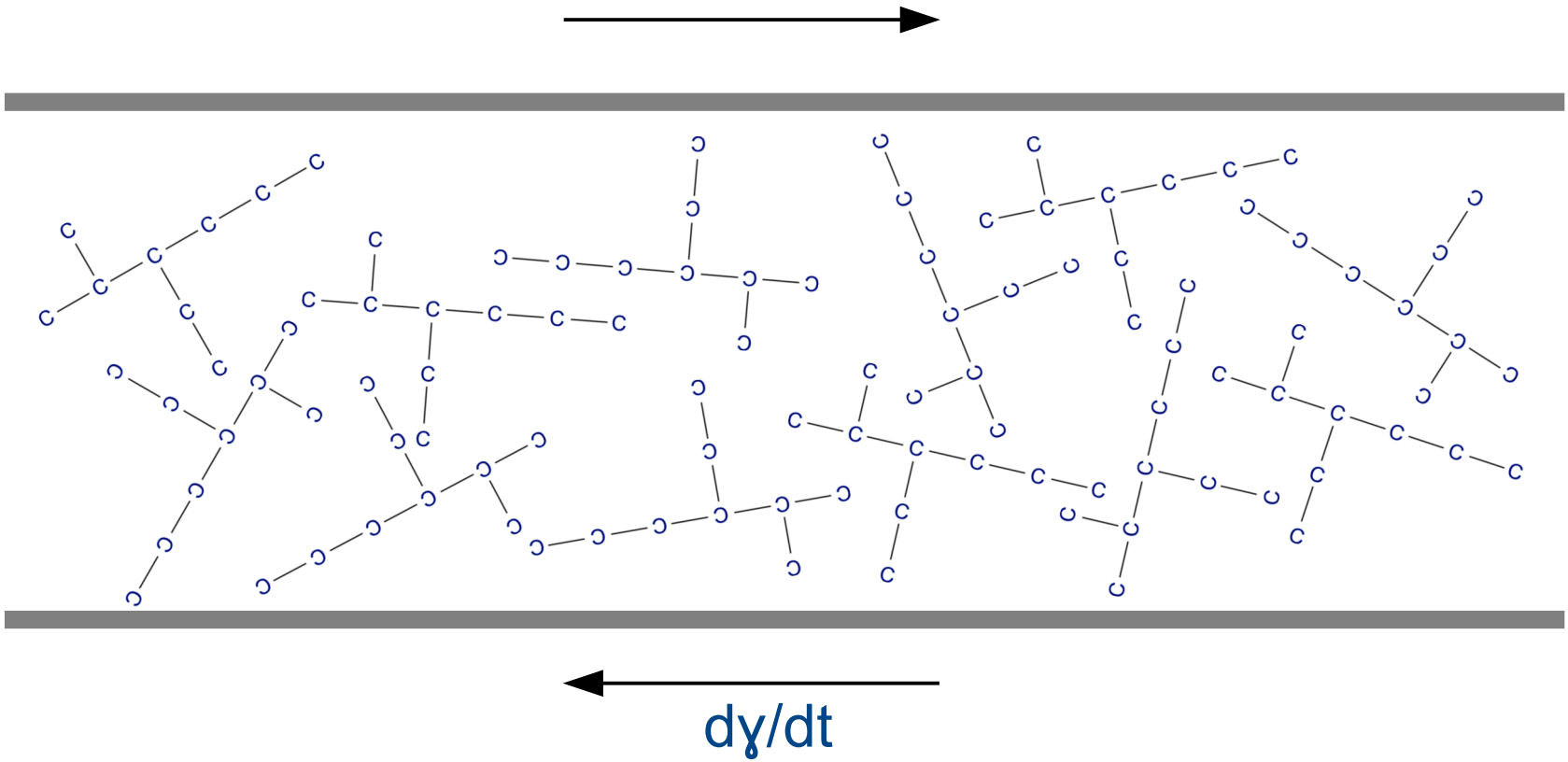
Free volume theory R^2=0.899

Summary of machine learning accuracies

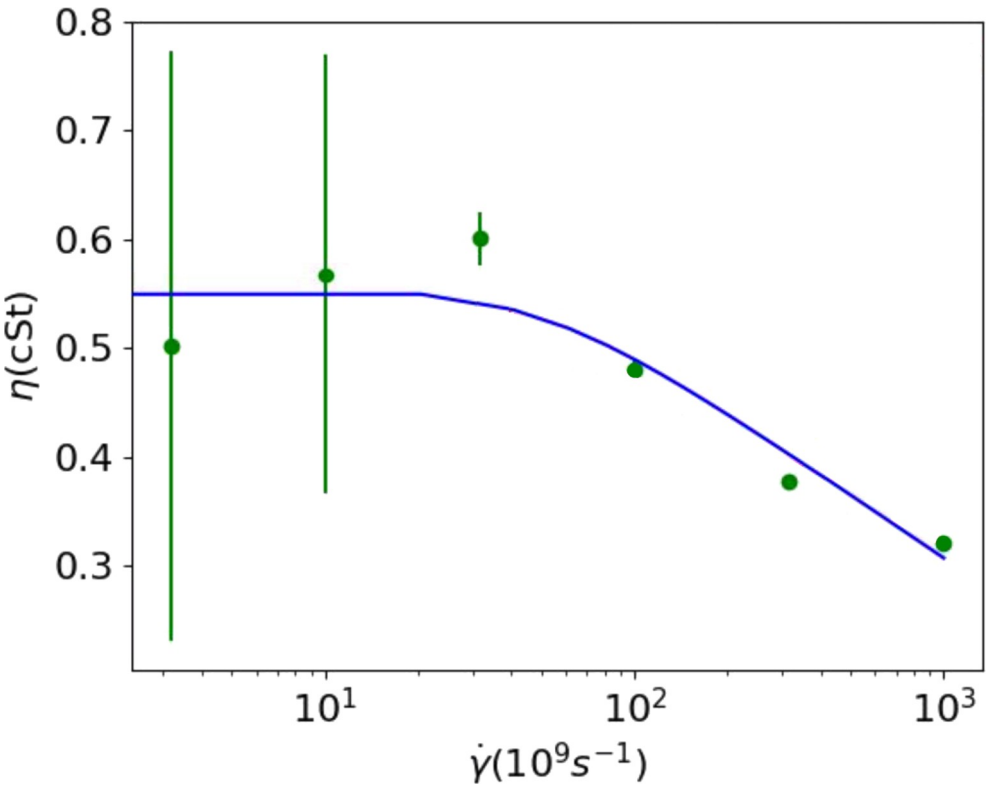
Property	Machine learning	Alternate
Density	0.987	0.890
Heat capacity	0.996	0.995
Vapor pressure	0.962	-
Flash point	0.997	0.971
Melting point	0.998	0.991
Boiling point	0.992	0.977
Kinematic viscosity	0.998	0.899

P. Santak & G.J. Conduit, Fluid Phase Equilibria 501, 112259 (2019)

Non-equilibrium molecular dynamics



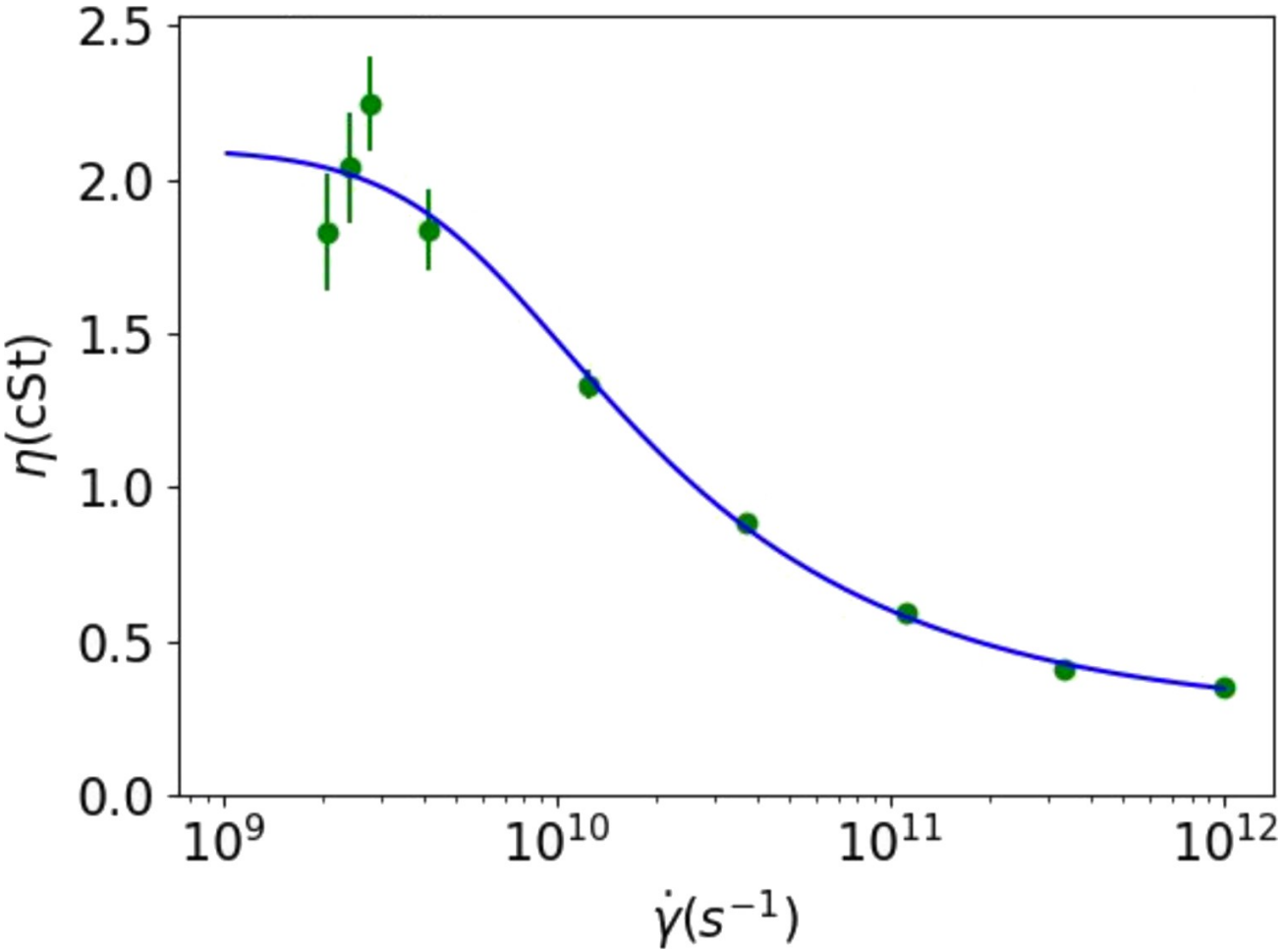
Kinematic viscosity of hexane



Increasing uncertainty on approaching zero shear rate

Carreau model guides extrapolation to zero shear rate

Viscosity of hexadecane at 60°C



Viscosity of straight chain alkanes

Hydrocarbon	20°C	40°C	60°C	70°C	100°C
Hexane	0.52 (0.56)	0.37 (0.37)	0.33 (0.34)	-	-
Decane	1.23 (1.27)	1.01 (1.00)	0.83	0.61	0.52
Tetradecane	2.93 (3.06)	2.04	1.51	1.27	1.02
Hexadecane	4.49 (4.51)	2.94 (2.92)	2.19 (2.06)	-	1.45 (1.41)

Comparison to other approaches

Hydrocarbon	20°C	40°C	60°C	70°C	100°C
Hexane	0.52 (0.56)	0.37 (0.37)	0.33 (0.34)	-	-
Decane	1.23 (1.27)	1.01 (1.00)	0.83	0.61	0.52
Tetradecane	2.93 (3.06)	2.04	1.51	1.27	1.02
Hexadecane	4.49 (4.51)	2.94 (2.92)	2.19 (2.06)	-	1.45 (1.41)

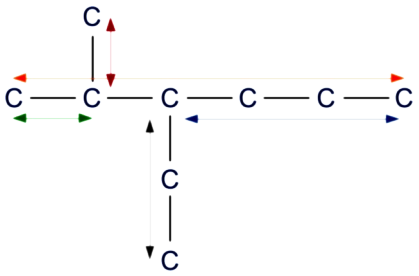
Our molecular dynamics R^2=0.95

Other molecular dynamics R^2=0.69

P. Santak & G.J. Conduit, accepted for Journal of Chemical Physics

Merge experiment & simulation with machine learning

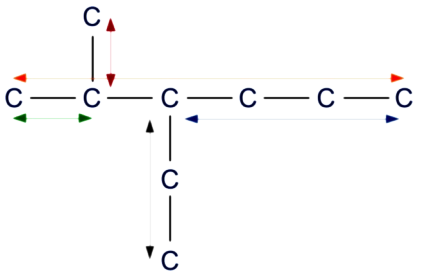
Structure



Properties

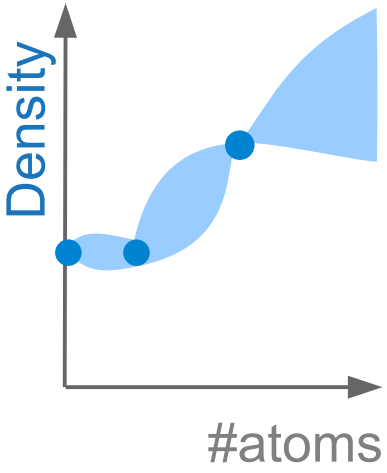
Merge experiment & simulation with machine learning

Structure

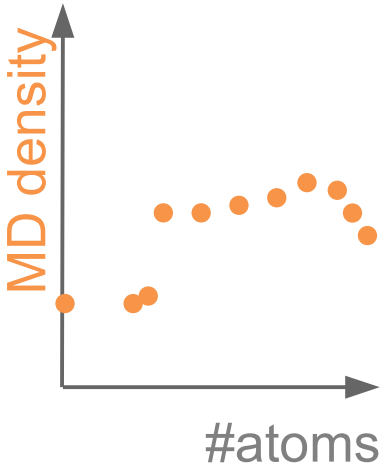


Properties

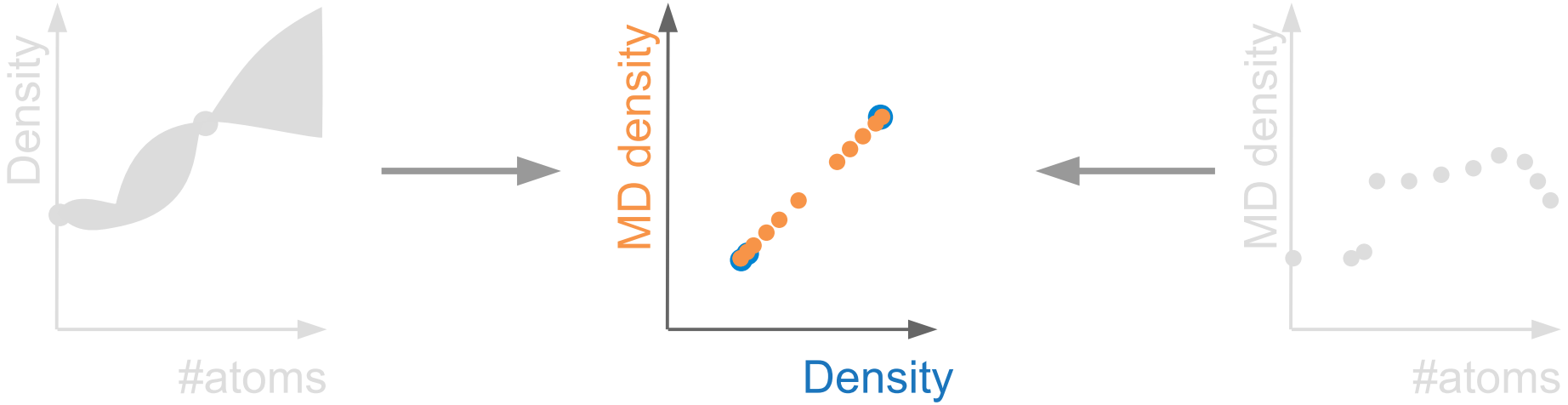
Insufficient data for density



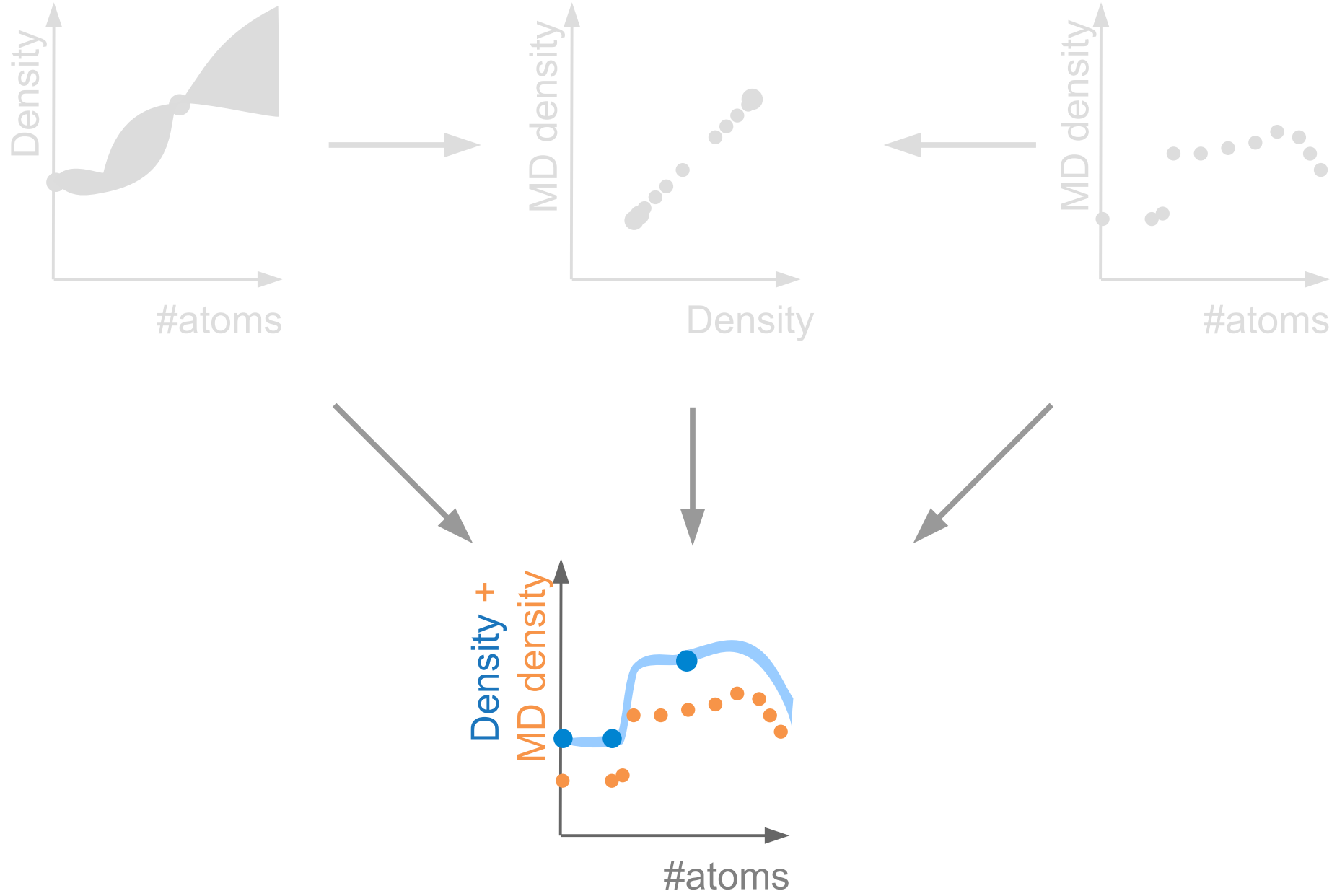
Molecular dynamics simulations capture trend



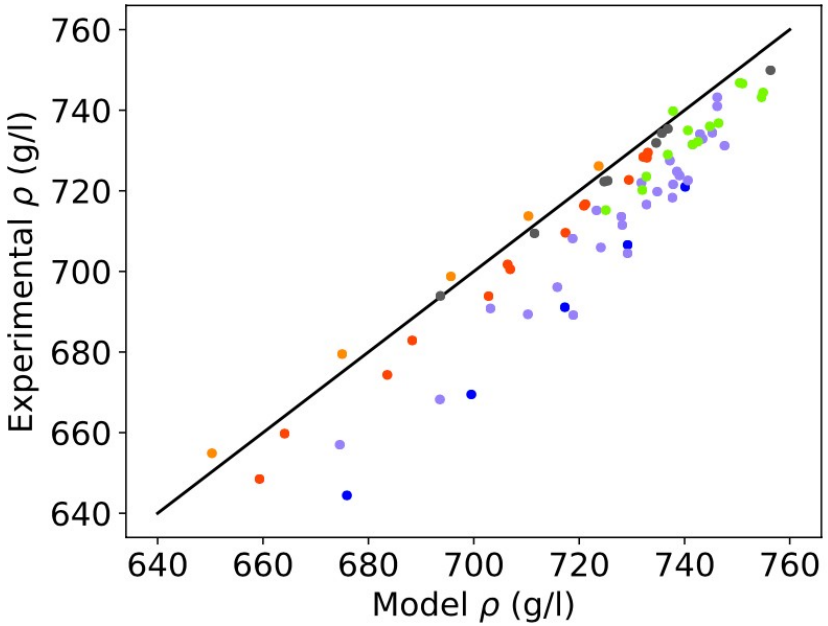
Simple relationship between simulation and experiment



Merging properties with the neural network

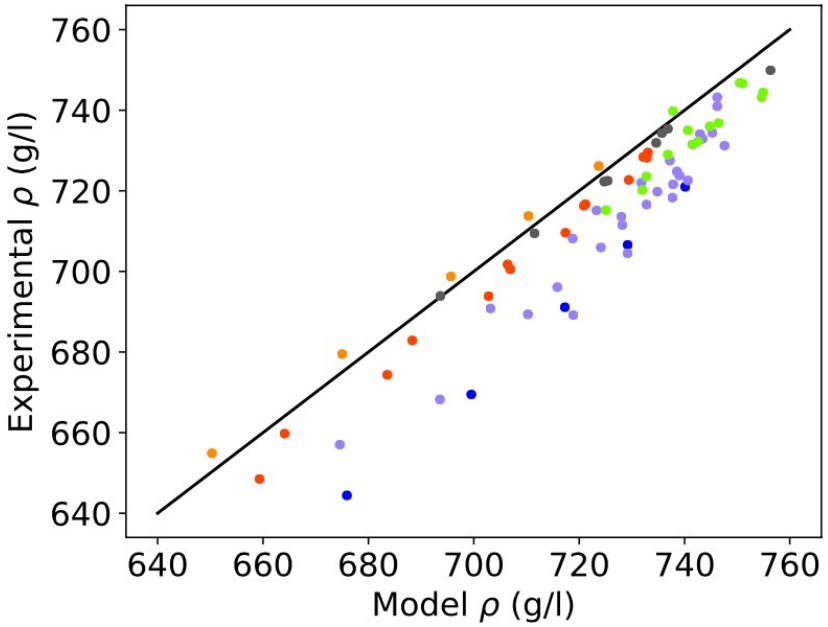


Performance before correction

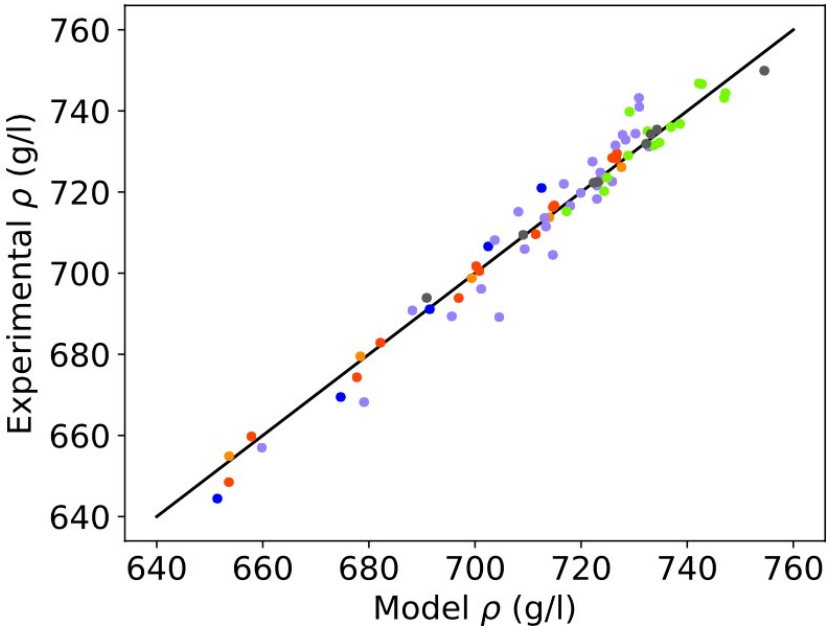


Linear alkane, methyl group, 2,2-dimethyl series,
ethyl-methyl group, other alkanes, other molecules

Performance with correction



$R^2 = 0.890$



$R^2 = 0.991$

Targets for a lubricant

Flashpoint	> 110°C
Viscosity	< 3.9cSt
Boiling point	> 250°C
Density	< 800mgmL^{-1}

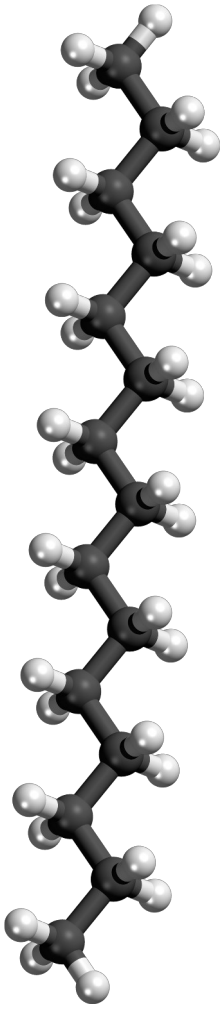
Designing a lubricant

Flashpoint = 122.55°C

Viscosity = 3.78cSt

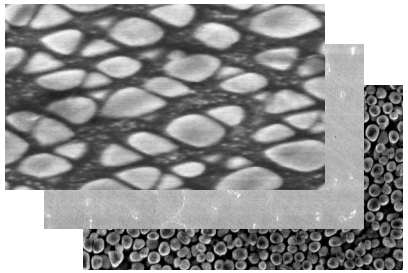
Boiling point = 270°C

Density = 769mgmL^{-1}



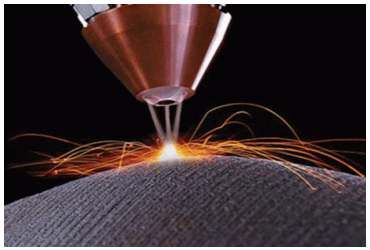
More materials designed

Nickel and molybdenum



Steel for welding

3D printing alloys



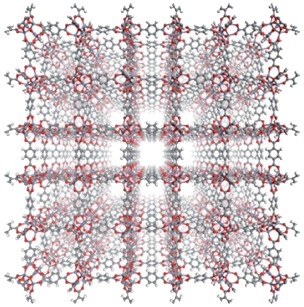
Experiment and DFT for batteries

Application to chemicals and drugs

Design concrete mixtures on site

BASF
We create chemistry

Metal organic framework



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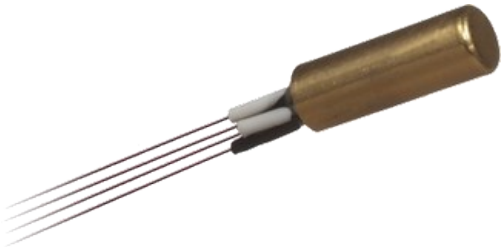
Thermometer



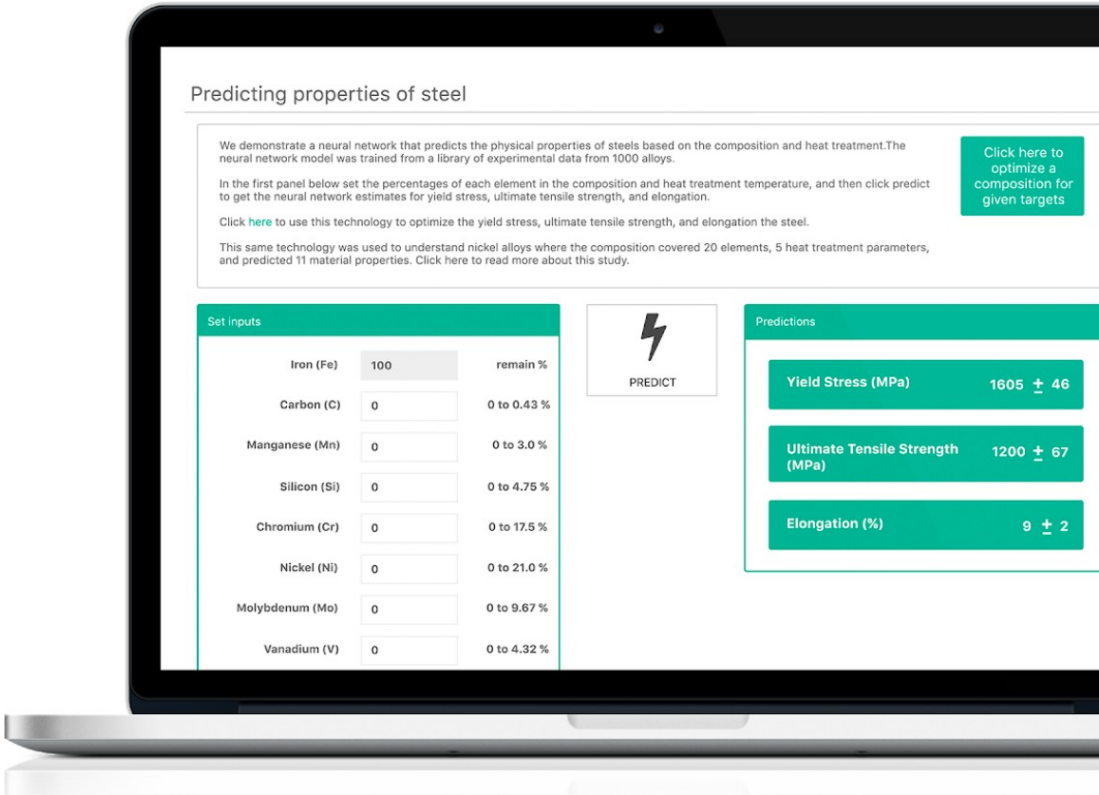
Cambridge Cryogenics

Drug design

e-therapeutics
optibrium
AstraZeneca
Celgene
Takeda
Constellation
PHARMACEUTICALS

Taken to market by Intellegens

1. Upload data
2. Train model
3. Predict & design



https://intellegens.ai

Summary

Model many physically relevant properties of lubricants with machine learning

Optimal strategy for non-equilibrium molecular dynamics simulations of viscosity

Merge computational and experimental data

Taken to market by Intellegens

P. Santak & G.J. Conduit Fluid Phase Equilibria 501, 112259 (2019)
P. Santak & G.J. Conduit, accepted for Journal of Chemical Physics