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Bristol Composites Institute

High-Throughput Computational Chemistry for Polymer Discovery

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UKRI Engineering and Physical Sciences Research Council

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Problems with Polymer Discovery

- Slow development cycle
- Random trial and error
- High financial and environmental cost

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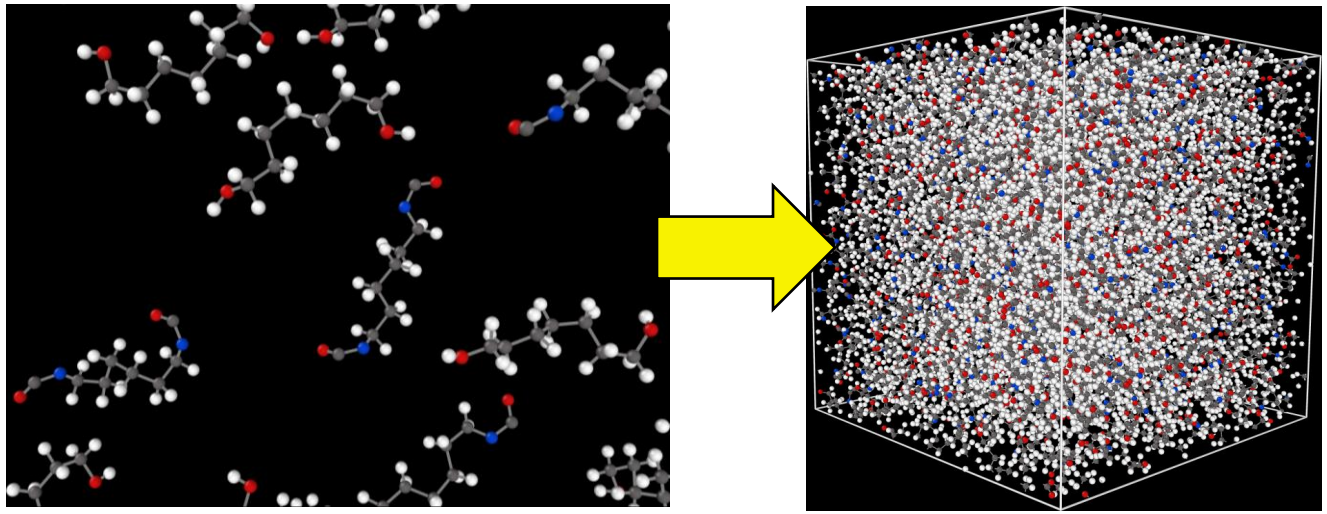
Molecular Dynamics

- Modelling chemistry using classical mechanics
- Model large repeating structures like polymers
- Enable rapid exploration of material design space



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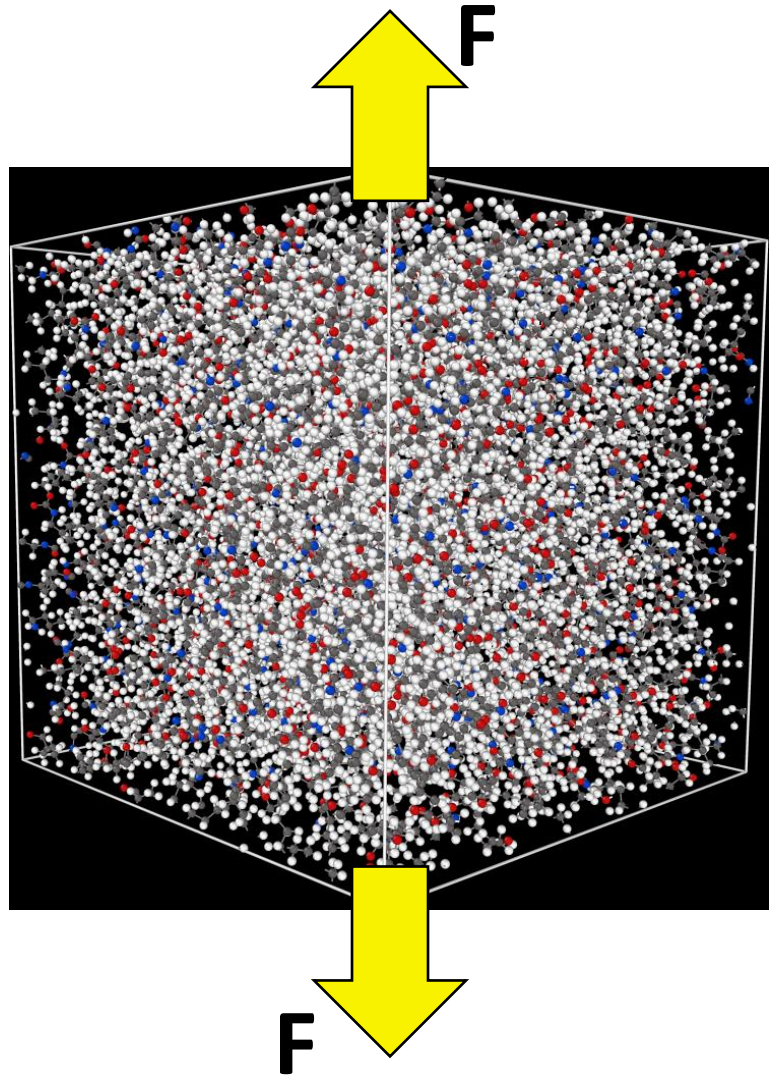
MD Predictable Properties

- Glass Transition Temperature (T_g)
- Storage & Loss Modulus
- Density and Free Volume
- Degree of Crosslinking
- Coefficient of Thermal Expansion (CTE)
- Young's Modulus
- Shear Modulus
- Poisson's Ratio
- Yield Stress



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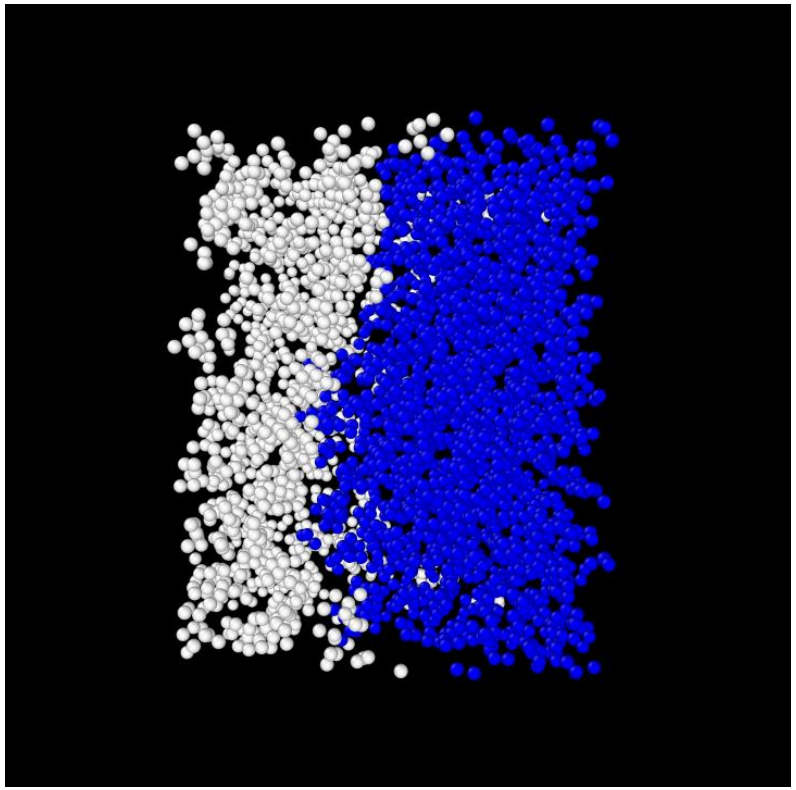
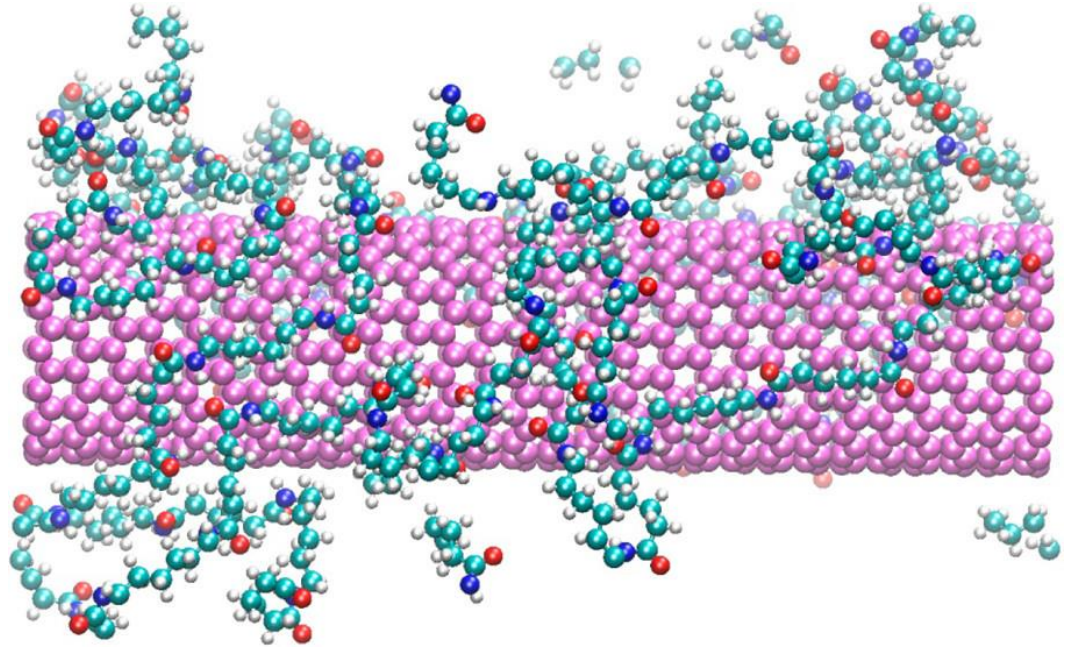
Atomistic Visualisation

Polymer/Solvent Phase Separation



Polymer/CNT Interface



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Welcome to Computational Chemistry!

This sounds too good to be true?

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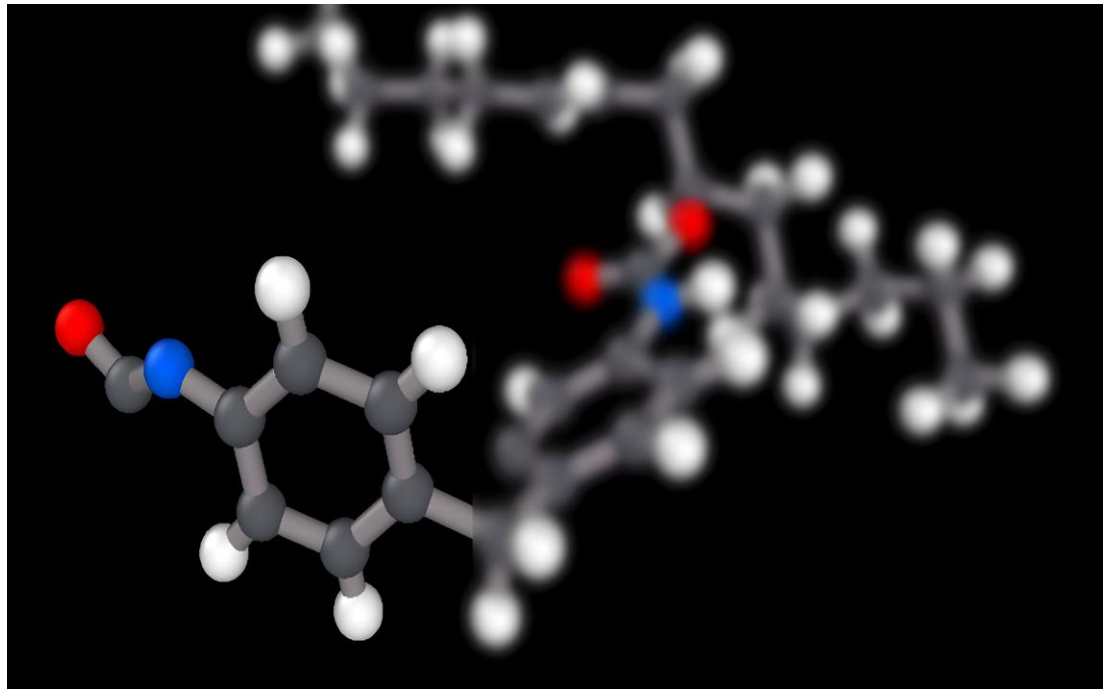
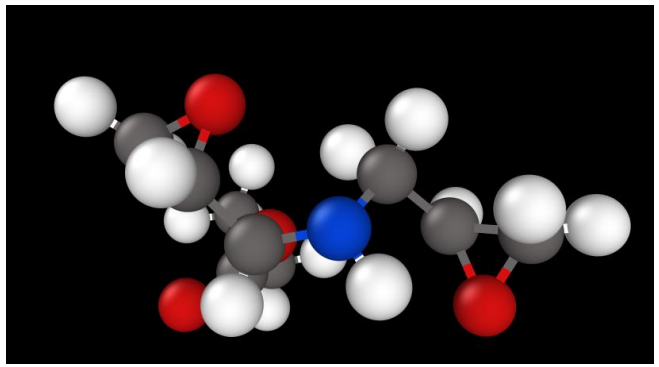
Problems with Computational Chemistry

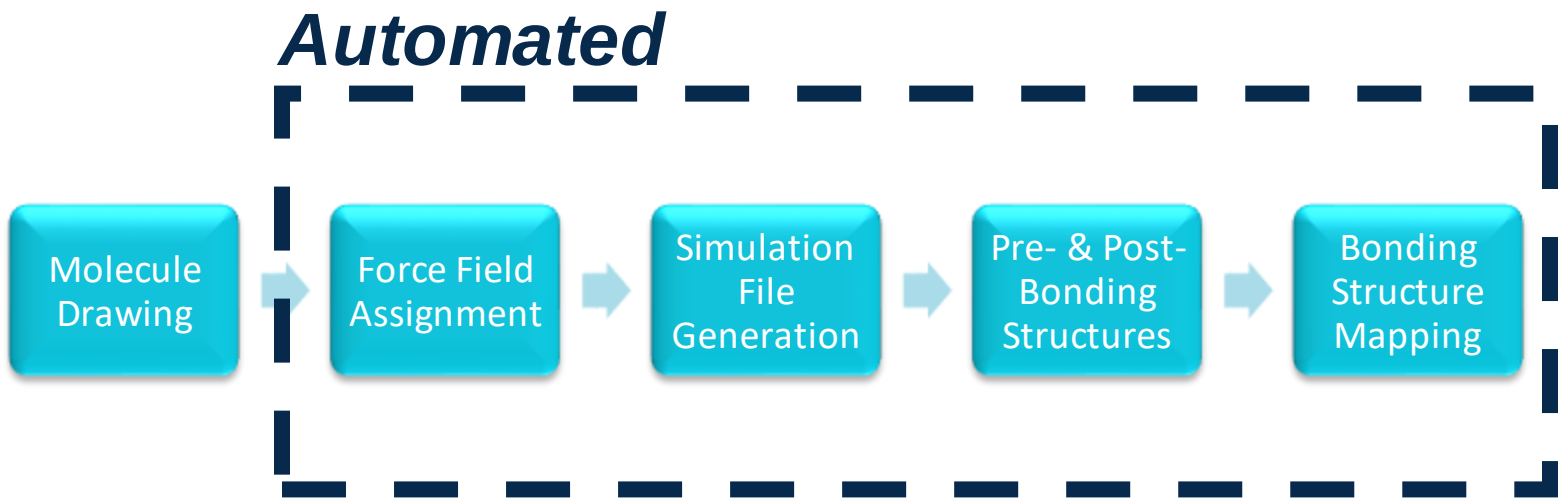
- Significant barrier to entry
- Difficult and tedious pre-processing
- High computational cost



Automated Pre-Processing

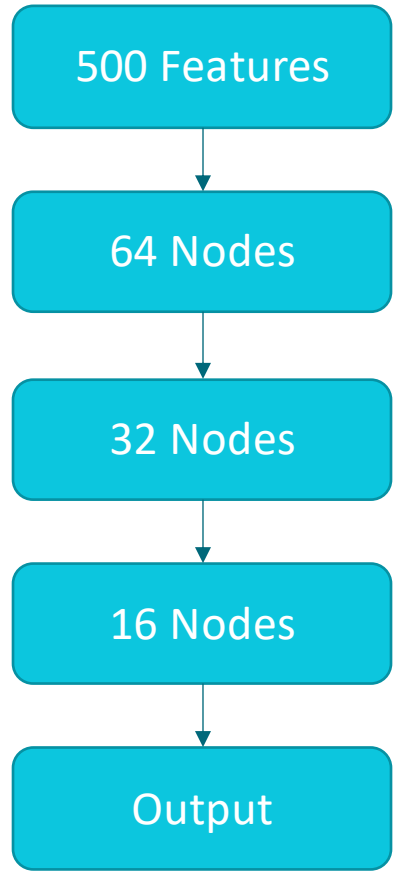
- Developed an automated pre-processing workflow
- Polymer models easily parameterised and built
- Only requires the user to draw the molecule





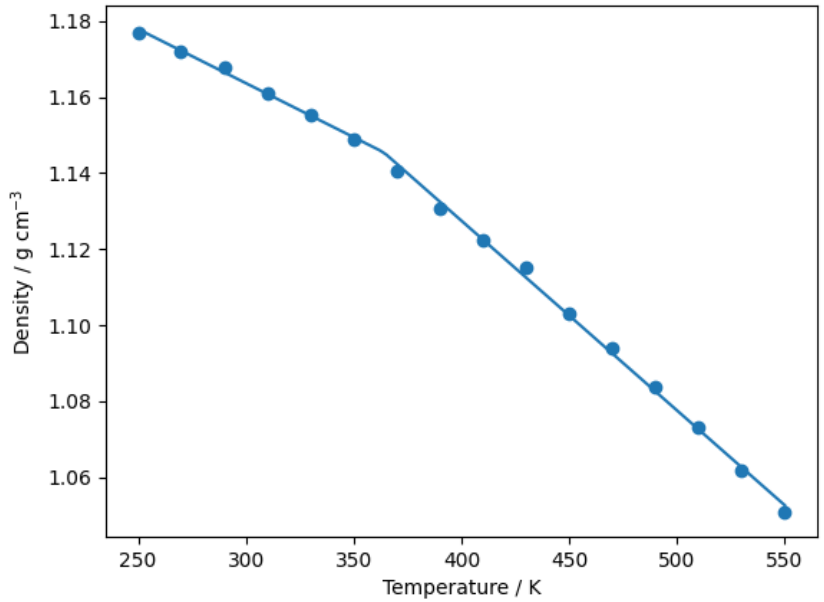
Fast Simulations - Machine Learning Surrogates

- Current MD simulations: 24 – 36 hrs
- Eliminate MD simulation through prediction
- Using small neural network architecture
  - Low computational cost to train



Glass Transition Temperature

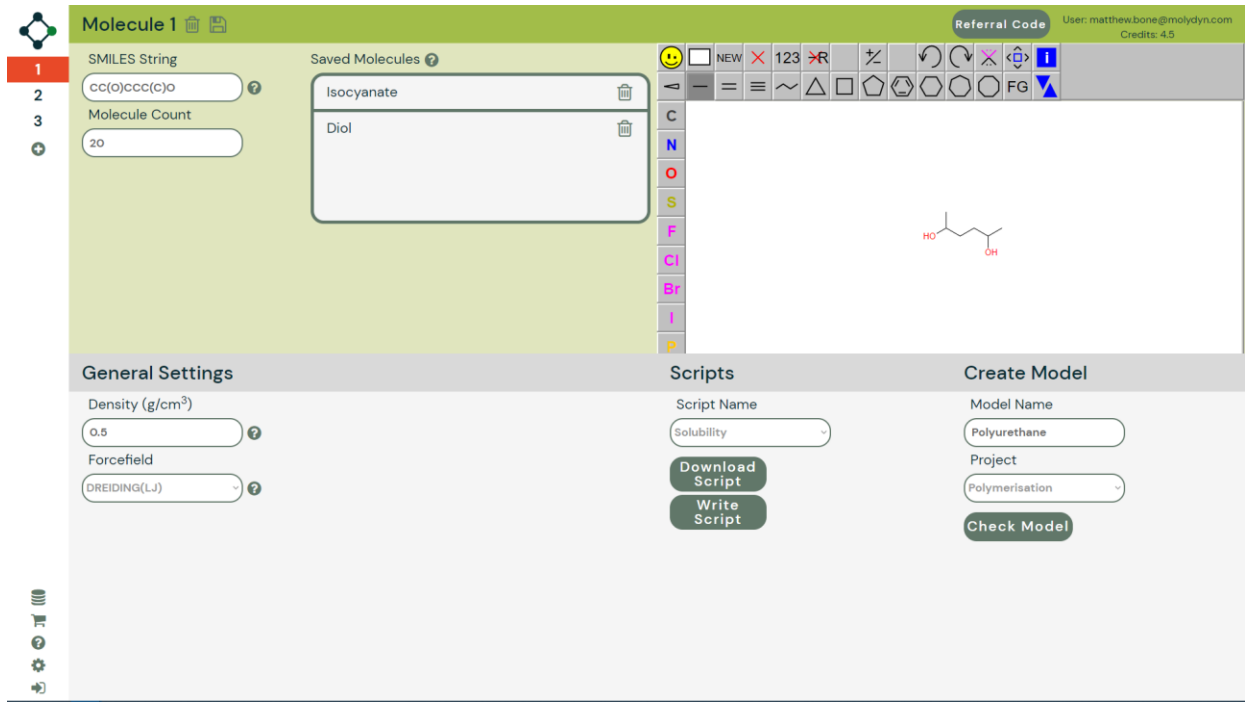
- 96 characterised polyurethane models
- T_g range 320 – 450 K
- Close prediction from simple feature
  - MAE: 10-20 K; RMSE: 20-30 K
- ML use significantly reduces runtime
  - 75% reduction



Commercialisation

- Accessible chemical simulation for everybody
- 90% reduction in pre-processing time
- Developing total simulation solution

Molydyn



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Questions?
Come find my poster!

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Acknowledgements

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