University of Bristol
Bristol Composites Institute (ACCIS)

ACCIS
ADVANCED COMPOSITES COLLABORATION FOR INNOVATION & SCIENCE

UKRI Engineering and Physical Sciences Research Council

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EPSRC Centre for Doctoral Training in Composites Science, Engineering and Manufacturing

Molecular Modelling for Materials Science

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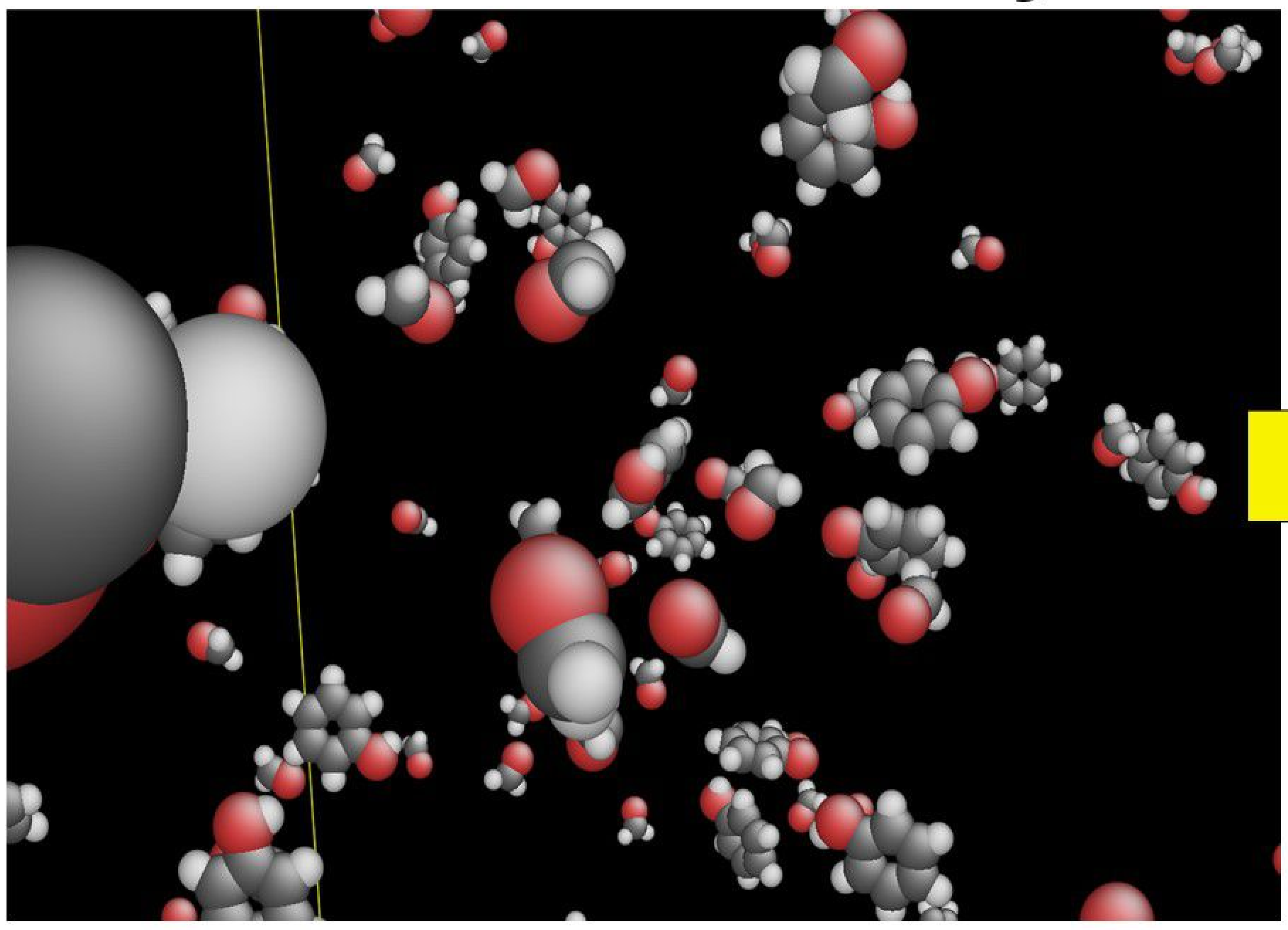
Introduction

Materials science is steadily adopting computational modelling simulations to accelerate and enhance the materials discovery process. Use of molecular dynamics (MD) is a core technique supporting this effort. MD allows the user to model chemical structures at an atomistic ($1x10^{-10}$ m) scale. Polymeric materials, nanofillers, and composites can all be modelled and analysed to determine physical, mechanical, and chemical properties. Integrating high throughput modelling with data science techniques, such as machine learning and artificial intelligence, enables rapid testing and optimisation of new materials. As materials become more complex, computer simulation becomes the only feasible way to fully explore the design space; simultaneously increasing the scope of potential materials whilst reducing development costs.

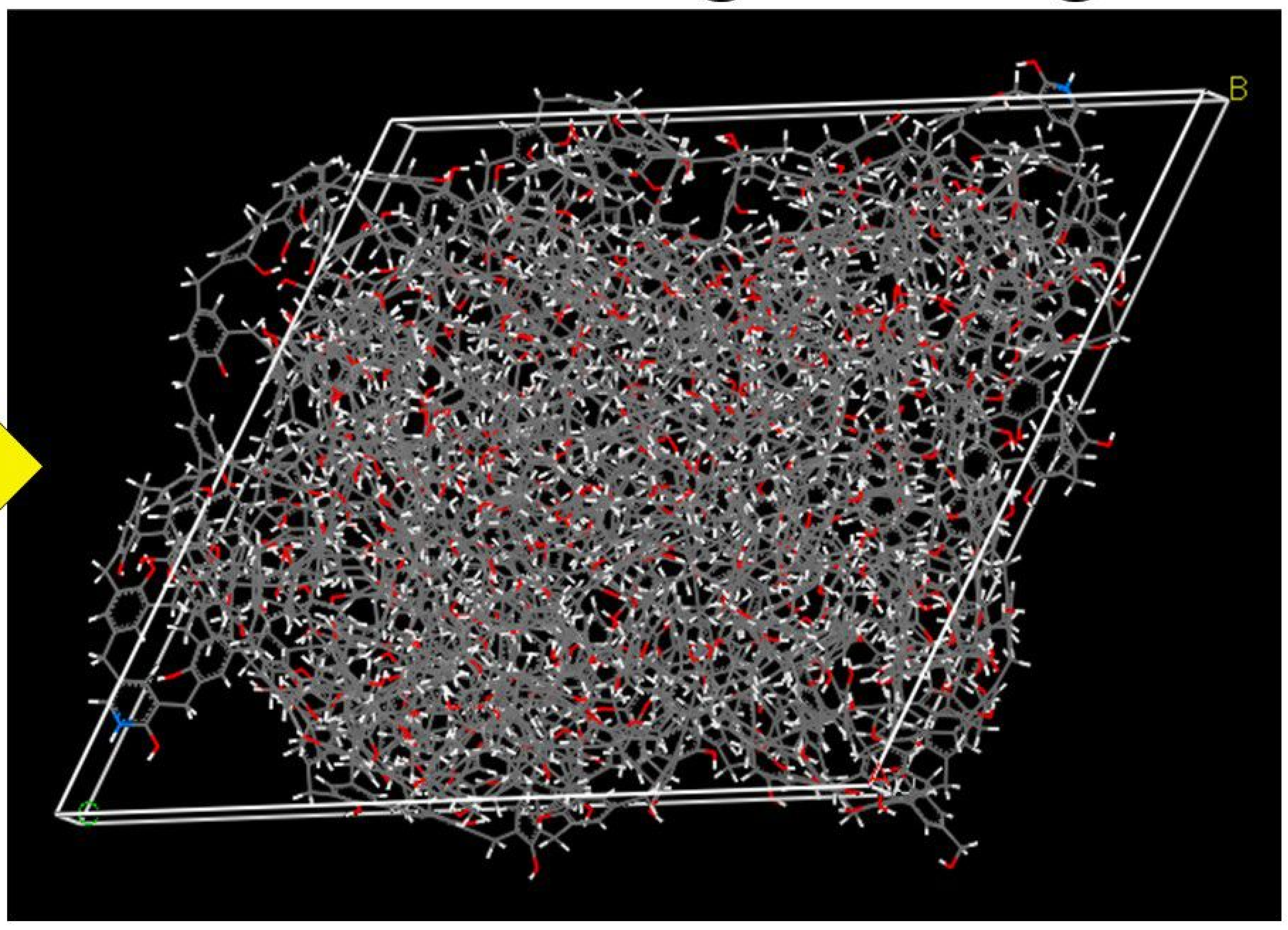
Virtual Chemistry



Chemical processes or experiments that can be modelled in MD:

- Atomistic Structure of Composites
- Polymerisation
- Chemical Reactions
- Reaction Profiles
- Solvation
- Crystallography
- Diffusion
- Chemical Potential

Practical Engineering

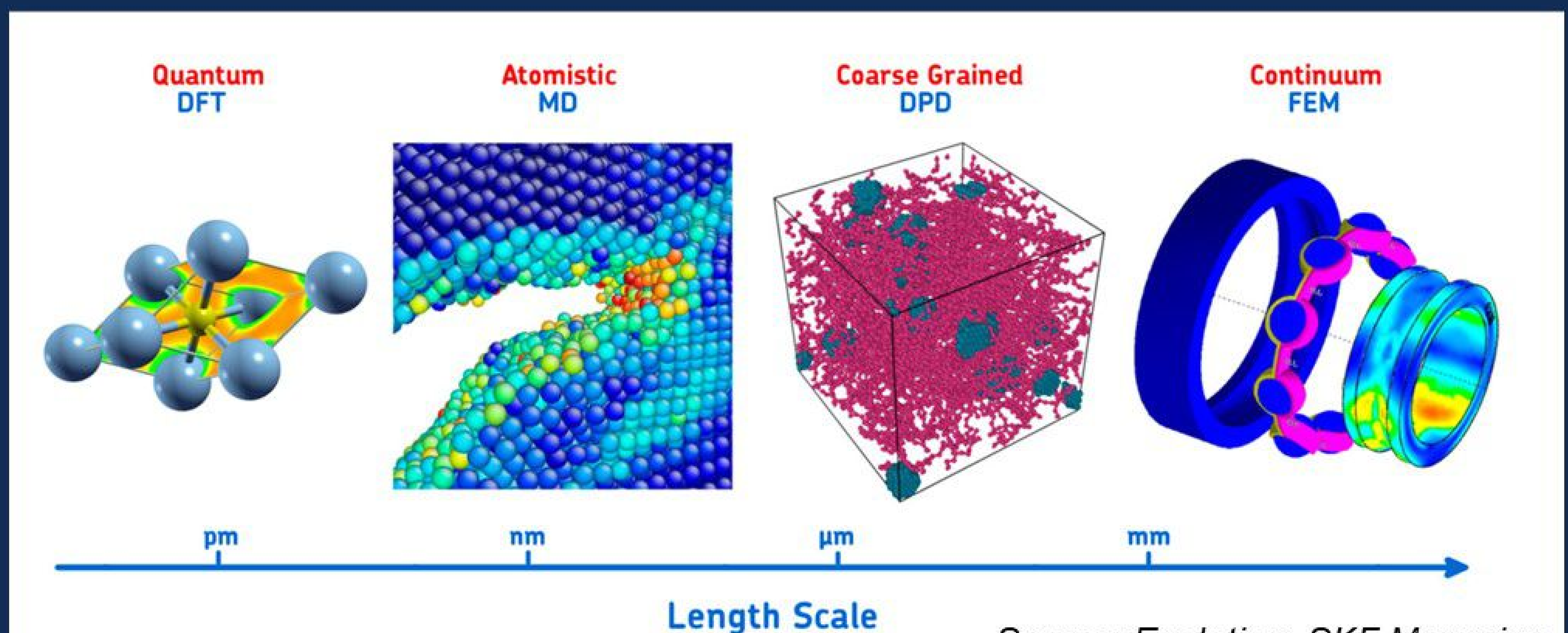


Example material properties that can be characterised from MD simulation:

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

Multi-scale Modelling

The next stage in computational materials science is incorporating simulation data across a range of modelling scales. This will enable development of large structures that are designed and optimised from an atomic level. Greater control of material properties will lead to bespoke materials that facilitate the next generation of structures.



Source: Evolution, SKF Magazine

Bone, M.A.; Macquart, T.; Hamerton, I.; Howlin, B.J., *Polymers* **2020**, *12*, 926.