us-eu bridging research efforts

Hybrid Modelling of Nanocomposite Properties

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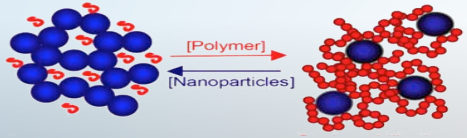
- In which areas are multi-scale and multi-physics approaches most advanced and could lead to a multi-purpose modelling platform?

- ***Dielectric Materials by Design:***
- *Nanodielectrics*
- *High Energy-Density capacitors for energy storage*

- ***Structural Materials by Design:***
- *Nanocomposites with tailored thermomechanical properties*
- *Materials with Pareto-optimized sets of properties*

Hybrid Modelling of Materials Properties



Nanoparticle dispersion in polymers

POLYMERS

NANOMATERIALS

Protein structure/function in nonaqueous/

Hybrid Modelling Challenge: How do we predict the properties of these new materials – in non-equilibrium conditions – due to manufacturing needs - using methods that are scalable, grounded in physics, and are not so slow or expensive that they are unfeasible?

Protein stabilization by nanoscale curvature

BIOMOLECULES

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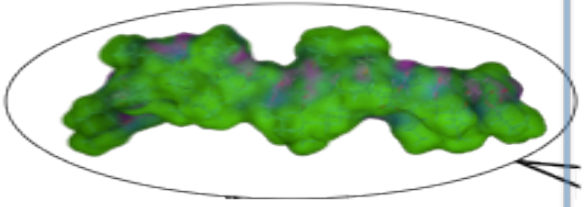
Example: A Hybrid Physics / Informatics Approach

MQSPR

Lone Pair Potentials
Hydrophobicity
Electron Density
Electrostatic Potential

Polymer Structure & Nanoparticle Surface Structure



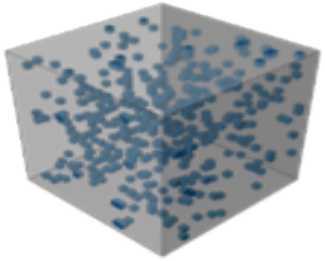
Surface Energies

γ^{polar}

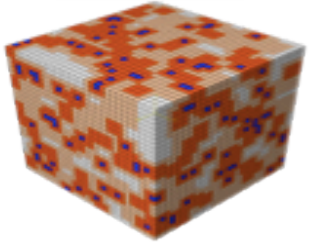
$\gamma^{dispersive}$

Interphase Chain Mobility

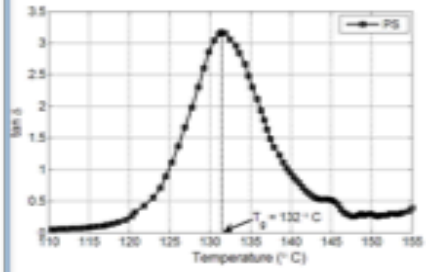
Particle Morphology



FEA



Thermomechanical Response



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Hybrid Modelling of Nanocomposite Properties: **Grand Challenges**

- On which **Grand Societal Challenges** would a *unified modeling platform* have the largest impact?
- ***health and well being?***
- ***secure, clean and efficient energy?***
- ***food security?***
- ***smart, green and integrated transport?***
- ***climate action?***
- ***resource efficiency?***
- ***raw materials?***

Hybrid Modelling of Nanocomposite Properties: **First Steps**

- In which areas would a **US-EU Collaboration** be most successful in the short to mid-term?
- *Integrating **nanomaterial property data** into a shareable database for model development and validation*
- *Establishing a joint initiative for linking different length scale modelling methods in a **multi-functional webtool***