

PHYSICS COLLOQUIUM: Simulations of Soft Materials - Identifying and Accessing the Key Length-Scales

Doug Cleaver Professor of Materials Modelling Sheffield Hallam University

About The Speaker:

My research is in the field of computer simulation of complex fluids and soft condensed matter. Much of my work has focussed on liquid crystalline behaviour, but more recently my interests have broadened to other selfassembling soft matter including polymers and deformable, supramolecular assemblies. An underlying theme is the use of computer modelling to investigate aspects of physically significant systems which are inaccessible to experimental and theoretical study. In many cases, achieving this has required working with collaborators from different disciplines and sectors. As well as being a research Professor, I am Director of my University's Doctoral School and am currently Chair of UKCGE, the UK's national representative body for postgraduate education and research.



Abstract:

The challenge - and the allure - of soft matter systems is the sheer range of time- and length-scales over which they operate. This provides rather a conundrum to simulation: choosing a model-type is a pre-requisite for generating results but it also effectively imposes a restriction on the set of phenomena that the resultant simulations will be able to access.

In this talk, two simulation studies of soft matter will be presented. The first relates to the glass transition of a polymeric binder (HTPB) and functionalised silica nano-cubes (POSS). The second investigates the hierarchical self-assembly of twisted fibres and tubules. Whilst both are based on similarly-sized molecular units, and metastability is a common theme, it transpires that their key length-scales are very different.



For more information, contact : Linda Hirst lhirst@ucmerced.edu

<u>Date:</u> 2/25/2022

<u>Time:</u> 10:30 AM - 11:50 AM

Location:

Please contact <u>snsgradstaff@ucmerced.edu</u> for the Zoom information.