MAXWELL INSTITUTE FOR MATHEMATICAL SCIENCES

THE UNIVERSITY of EDINBURGH

HERIOT WATT UNIVERSITY

A Maxwell Institute Colloquium

Realistic simulations of the molecular organization in thin organic films

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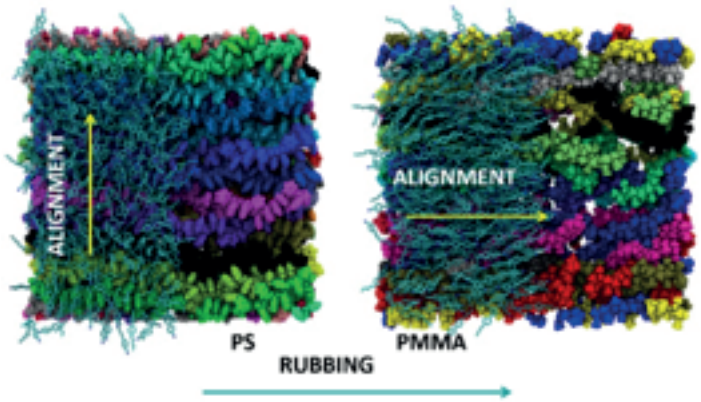

Organic functional materials (liquid crystals and organic semiconductors in particular) are key components of displays and organic electronic devices where they are inevitably employed in very thin (nano to micron scale). Information on their surface alignment and anchoring, although essential for these applications, has been supplied only empirically, rather than obtained bottom up from the molecular level. Atomistic simulations are changing this. In the talk we show examples of the prediction of alignment and anchoring of organic functional materials at the interface with different hard and soft substrates. The importance of the film fabrication process on molecular alignment is also briefly discussed taking as examples the vapour deposition of pentacene on fullerene and silica.

Location: 5.02, 5th Floor, ***Thomas Bayes Centre***
Time: 3:30-4:30, March 29, 2019

A reception will be held following the talk