SYUK 1: United Kingdom as Guest of Honor I

Time: Wednesday 9:30–12:15 Location: H2

Invited Talk SYUK 1.1 Wed 9:30 H2

Structure and Dynamics of Interfacial Water — •Angelos Michaelides — University of Cambridge, Cambridge, UK

There are few molecules, if any, more important than water. However, remarkably little is known about how it interacts with surfaces, particularly at the molecular level. In this talk I will discuss some of our recent work on the application and development of a variety of state of the art computer simulation methods to better understand the structure and dynamics of water at surfaces and under confinement. Specific topics discussed will include work carried out in collaboration with experimentalists to understand the growth and diffusion of ice clusters at metal surfaces, heterogenous ice nucleation, and water confined within 1- and 2-dimensional membranes. Methodological developments aimed at providing more accurate treatments of adsorption on and bonding within solids will also be covered, as well as an efficient machine learning strategy for simulating complex aqueous interfaces.

Invited Talk SYUK 1.2 Wed 10:00 H2

A molecular view of the water interface — •Mischa Bonn — Max Planck, Mainz, Germany

Water surfaces and interfaces are ubiquitous, not just in nature, but also in many technological applications. Water is a rather unique liquid, owing to its strong intermolecular interactions: strong hydrogen bonds hold water molecules together. At the surface of water, the water hydrogen-bonded network is abruptly interrupted, conferring distinct properties on the interface, compared to bulk. I will present some challenges and progress in the study of interfacial water. Specifically, I will address how to study the ~1 monolayer of water molecules that is in direct contact with the other phase, and distinguish this ~Angstrom-thin layer from the bulk. The question rises how large the interface is. And can we describe the interfacial region as a modified dielectric continuum, or do we need to consider molecular structure?

Invited Talk SYUK 1.3 Wed 10:30 H2

Motile cilia waves: creating and responding to flow — •Pietro Cicuta — University of Cambridge, Cambridge, UK

Motile cilia are active filaments present on the surface of various human organs, where they perform crucial functions by driving surface flows. Structurally, they are conserved across the eukaryotes. Cilia can affect each other, for example leading to phase locking of their beating, by the forces they exert on each other through the fluid and in some cases through the cell cytoskeleton.

Some beautiful physics has been developed by various teams in the last decade to understand how the details of beating on each cilium can lead to specific phase locking, and to the emergence of collective waves. In recent work we have explored the role of external flows, both oscillatory and constant. Analogies can be drawn between these flows and the effect of external magnetic fields in magnetic systems.

We present both experimental results, and numerical explorations of a simple class of "rower" models of motile cilia.

Invited Talk SYUK 1.4 Wed 11:00 H2

Cilia and flagella: Building blocks of life and a physicist's playground — •Oliver Bäumchen — Chair of Experimental Physics V, University of Bayreuth, Bayreuth, Germany

Flagella and cilia are actively beating, hair-like cellular appendages that represent universal building blocks of life. They inherit various essential functions that range from driving fluid flows in the mammalian brain and transporting mucus in the respiratory tract to realizing microbial motility and navigation through complex environments. While large-scale flows are achieved through the coordination of dense ciliary carpets, only a few isolated flagella are needed in order to propel a single-celled microorganism. These flagella displace the surrounding fluid by means of periodic motions, while precisely timed modulations of their beating enable the cell to steer towards or away from specific locations. In this presentation I will focus on the interactions of flagella with interfaces and elucidate how physical principles advance our understanding of microbial motility and emergent phenomena in microbial suspensions. Microorganisms that are equipped with photoreceptors may adapt their flagella beating and also actively switch their flagella-surface interactions in response to light cues. These skills allow photoactive microorganisms to effectively adapt to variable light conditions in their natural habitats and make flagellated microbes a fascinating playground for physicists.

15 min. break

Invited Talk SYUK 1.5 Wed 11:45 H2

Computational modelling of the physics of rare earth - transition metal permanent magnets from $SmCo_5$ to $Nd_2Fe_{14}B$ — •Julie Staunton — University of Warwick, Coventry CV4 7AL, U.K.

Magnetic materials are ubiquitous, technologically indispensable and a deeper understanding of the physics is needed for the design of new permanent magnets. Most strong magnets contain both rare earths (RE) and transition metals (TM) and this talk will describe recently developed *ab initio* modelling of intrinsic properties. Each RE atom has a magnetic moment, set up by its nearly localised f-electrons, immersed in a glue of septillions of valence electrons coming from all the RE and TM atoms. Local magnetic moments associated with the TM atoms also emerge from this complex electron fluid. The magnetic properties stem from the behaviour of the RE and TM local moments, the atomic arrangements and on the overall response to applied fields. *Ab initio* Density Functional Theory-based Disordered Local Moment (DLM-DFT) theory provides a parameter-free, accurate account of the electrons and incorporates the effects of the fluctuating local moments by averaging over them to describe temperature dependent effects. After demonstrating the computational modelling with calculations of the light RE-Co_5 permanent magnet class, the rich and complex behaviour associated with the Fe atoms in $Nd_2Fe_{14}B$ will be described together with its role in determining the hard magnetic properties of this champion magnet.