

Honours Student Presentations

DATE: Friday, March 11, 2022

TIME: 4:00 PM

PLACE: Webex

Speaker: Cassandra Clowe-Coish

Title: Computer Simulation of Dipolar-Depletion Colloids

Abstract: An experimental colloid-polymer mixture with an applied external electric field is subject to an induced dipole interaction and an apparent attraction due to depletion of solvent in close-approaching colloidal spheres. The electric field strength and polymer concentration affect the strength of these interactions and thus lead to manifestation of distinct phase transitions and, more generally, a variation in local order with these parameters. A computational system replicating the experiment is developed to examine the static properties of the colloid, with increased visual resolution in the direction of polarization and increased control of parameters. Such an approach is adopted to attempt to resolve the question of decreased local order at high polymer, high-field state points past a certain threshold, before which local order was observed to increase.

Speaker: Andrew Hadfield

Title: Effects of Macromolecular Crowding on Intrinsically Disordered Proteins

Abstract: A regular globular protein is composed of a chain of amino acids, and usually has one native structure. Intrinsically disordered proteins lack a native structure and can populate many different forms, making them ideal for binding. My project is to develop a coarse grain computational model of an IDP known as α synuclein, which is found in the brains of Parkinson's disease patients. α synuclein is a 140 amino acid length protein, and will be modeled using Langevin Dynamics. This model will then be fit to experimental data using scaling and shifting factors. The Radius of Gyration from this model that fits best will be used in order to study how the protein is affected by the introduction of the crowder polyethylene glycol. Crowders are used to simulate effects of the jam packed environment of living cells, rather than an open "test tube". The Radius of Gyration of α synuclein is decreased as the concentration of added crowders increases.

Speaker: Liam Newhook

Title: Marginally Outer Trapped Surfaces in Reissner-Nordstrom Spacetime

Abstract: Looping marginally outer trapped surfaces (MOTS) have been found and seem to be a key phenomenon during binary black hole mergers. These looping surfaces were then found in simpler Schwarzschild black holes in Painlevé–Gullstrand coordinates. The results presented in this talk show fascinating observations of looping MOTS in charged, Reissner-Nordström black holes, where we find looping, cusping, and oscillating MOTS behavior depending on the charge and stability of the black hole.

Speaker: Yimiao Zhao

Title: Suitability of Graphene monolayer as sensor for carcinogenic heavy metals in water

Abstract: The presentation will discuss the sensing ability of graphene monolayer for the detection of carcinogenic heavy metals like Arsenic (As), Cadmium (Cd), Chromium (Cr), Mercury (Hg) and Lead (Pb) in water and responsible for some disease. The Density functional theory has been used to perform the calculations of electronic properties to understand the sensing ability of graphene towards the heavy metals both in vacuum and aqueous environments. The variations in binding energy, density of state, HOMO and LUMO characteristics shows that graphene is a candidate of the detection of heavy metals.

ALL ARE WELCOME!