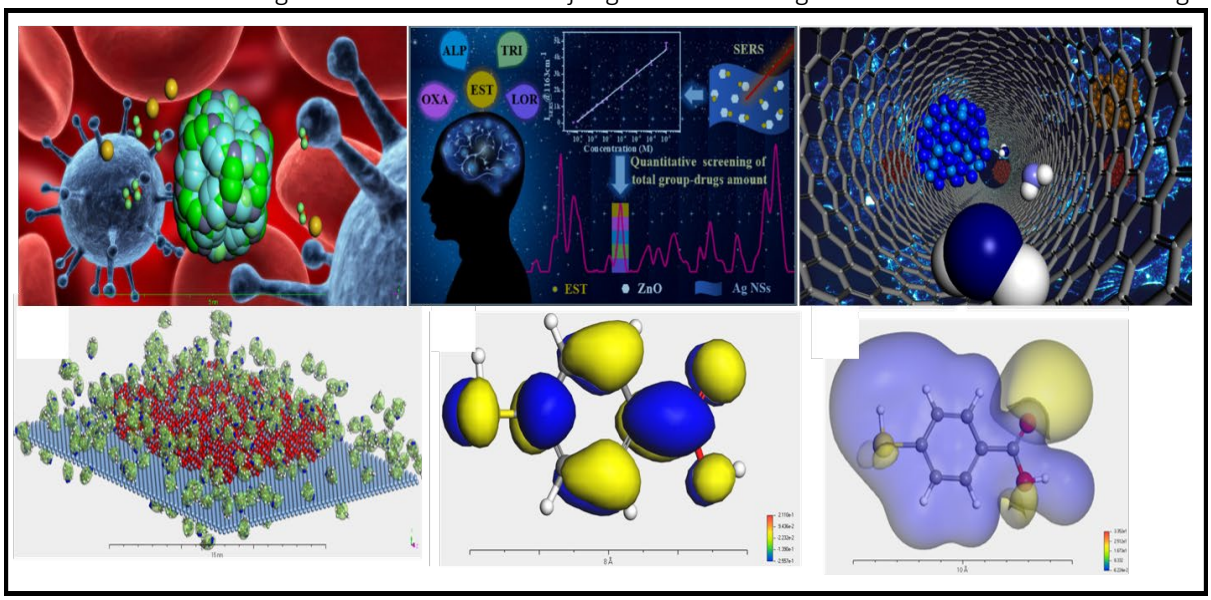
Nanomaterials for Health

In my research, through computational modelling, simulations and complimentary experimental work, I investigate the synthetic chemistry, magnetic characterization and biological applications of inorganic/organic - core/shell Fe_xO_y based magnetic nanoparticles as well as metal- and metal-oxide nanoparticles. Furthermore, I investigate the adsorption of different chemotherapy drugs and their concentrations onto Fe_3O_4 nanoparticles (to be employed as nanocarriers) within a Molecular Dynamics framework and Monte Carlo simulated annealing scheme. Bonding modes are investigated with reference to chemisorption, physisorption as well as hydrogen bonding in the context of bond strength (binding energy) as a function of both the drug molecule's loading as well as a change in nanoparticle size. Density functional theory (DFT) simulations are also performed to investigate the conditions for charge transfer from the temozolomide surfactant via the highest occupied molecular orbitals (HOMO), lowest unoccupied molecular orbitals (LUMO) as well as the electrostatic potentials. From this the preferential sites for both electrophilic and nucleophilic attacks can be calculated. This is important, for example, when considering the interaction with the blood-brain barrier as this remains a major challenge in effective chemotherapy of brain metastases. Despite the variability in its barrier function within brain tumour lesions, most drugs are still prevented from effectively entering the brain. With our computational studies, we investigate the changes the chemotherapy drugs may undergo when interacting with the nano-drug-carrier, within the context of delivering it to the target area. We also investigate the detection of small molecules and the screening *via* SERS of various drugs to create an accurate judgement in emergent medical and forensic settings.



Quantum-materials for Energy & Micro-technologies.

Quantum-wells and -wires are a type of two- and one-dimensional structure which are extremely small in diameter. When their physical dimensions are in the order of hundreds of nm to only a few nm, these structures are called nanocrystals(NCs). NCs may be engineered into different types of one-dimensional architectures like nano- wires, - rods, - tubes and - belts. In the case of two-dimensional structures, they are known as quantum-wells. Materials engineered and synthesized into (NCs) exhibit different properties from their bulk counterparts, partly due to their increase in surface-to-volume ratio, and partly due to quantum confinement effects that alter their density of electronic states. Therefore, these types of NCs display different electronic properties when their dimensions are altered. In the case of nanowires, by altering their length as well as their widths, these structures' electronic properties may be enhanced. Semiconducting NCs have distinctive physical and optical properties that

make them ideal candidates for future electronic and optoelectronic devices Candidate materials have shown remarkable promise in making progress towards efficient solar energy harvesting and conversion to electrical energy. However, improving the efficiency of these solar devices still requires much work. It is therefore (globally) an ongoing field of research. Quantum devices such as quantum-wells, wires and dots are promising candidates for future energy applications. Photovoltaics and supercapacitors are two possible routes through which the demand for higher efficiency energy generators and storage mechanisms may be satisfied. In my most recent research *via* both computational-modelling-and-simulations as well as through complementary experimental work like *electron beam lithography*, we are developing a quantum well device that acts as both a photovoltaic cell as well as UV-detector.