Application for a TSM-DTC funded PhD studentship

Please complete this form electronically
and submit to Lilian Wanjohi (l.wanjohi@imperial.ac.uk)
by Friday January 8, 2010

1st supervisor
Name: Prof. A.A.Kornyshev
CID (IC only):00331913
Institution, Department, Address: Imperial College London, Department of Chemistry, Chem.1 Bldg., SW7 2AZ London
Email: a.kornyshev@imperial.ac.uk
Phone: 020 759 45786

2nd supervisor
Name: Dr F.Bresme
CID (IC only):170551
Institution, Department, Address: Institution, Department, Address: Imperial College London, Department of Chemistry,
Chem.1 Bldg., SW7 2AZ London

Email: F.Bresme@imperial.ac.uk
Phone:0207 594 5886

3rd supervisor (optional)
Name:Dr A.Horsfield
CID (IC only): 523934
Institution, Department, Address:Department of Materials, Imperial College London
Email: ahorsfield@imperial.ac.uk
Phone: 0207 594 6753

Please complete the following:

1. Project title

Electrovariable nanoplasmonics: physics underpinning smart windows and mirrors

2. Project abstract (≤ 200 words please and please add 1 or 2 key references)

A new system has been recently suggested and described for electrically tuneable reflection of light at liquid-liquid interfaces [1]. It operates by using the voltage controlled adsorption and desorption of metal nanoparticles at the interface between two immiscible electrolytic solutions. With properly selected size and charge of nanoparticles and concentration of electrolytes, this system requires only a 0.5 V change in applied voltage to convert this interface from a transparent window to a mirror, and vice versa. The principle can be extended to solid/liquid electrochemical systems using transparent ITO electrodes. A preliminary theory of this phenomenon has been developed [1] which opens avenues for experimentation and more detailed theory. There is a group of experimentalists at Imperial already involved in this research

(Prof. A. Kucernak, Dr. J. Edel). The theory needs to move from being phenomenological to being microscopic using molecular dynamics / mesoscopic simulations [2] and electron density functional theory. The work includes: (i) developing a detailed theory of voltage controlled adsorption-desorption of nanoparticles beyond the mean field [3]; (ii) establishing a theoretical foundation for the design of nanoparticles with the required plasmonic spectral features ('beyond silver': low dissipation, with the plasma frequency in the far ultraviolet, and shifted to the visible range when forming a layer); (iii) constructing a detailed description of the dynamics of the loading and unloading of the interfacial layer with nanoparticles; (iv) going beyond the dipolar approximation in the description of optical properties of dense nanoparticle layers. The theory will be developed in close cooperation with the experimental work.

[1] M.Flatté, A.A.Kornyshev, M.Urbakh, Electrovariable nanoplasmonics and self-assembling smart mirror, (feature article), *J.Phys.Chem. C*, will appear on the web in January, printed –in February 2010.

[2] F. Bresme and M. Oettel, Nanoparticles at fluid interfaces, J. Phys. Condens. Matter, 19 413101 (2007).

[3] M.E.Flatte, A.A. Kornyshev, M Urbakh, Nanoparticles at electrified liquid-liquid interfaces: new options for electro-optics, Faraday Discuss. 143, 109-115 (2009);Giant stark effect in quantum dots at liquid/liquid interfaces: a new option for tunable optical filters, Proc. Natl. Acad.Sci USA, 105 , 18212-18214 (2008).

3. What is the multi-scale nature of the project? (≤ 100 words please)

This is an intrinsically multiscale problem. Starting from the electronic degrees of freedom that control the palsmonic spectra (sub nanometer length scale), to the nanoparticle self-assembly at the liquid-liquid interfaces, which cover length scales from nanometer – single particle problem – to micrometer (nanoparticle monolayers and the characteristics of the reflected light. As a theoretical background to prototype devices, the whole thing should end up with 1 cm^2 mirror. Covering these wide range of length scales which span at least 6 orders of magnitude requires the concerted effort of different levels of theory: from electronic computations and atomistic approaches to design of single particles with the specifically required plasmonic spectra and interfacial adsorption energies, to mesoscopic simulation and theoretical approaches to enable predictive studies of the structure and dynamics of nanoparticle assemblies. The dynamic range of the phenomena under study will span from electrical double layer relaxation 10^{-8} s to the target time of mirror operation, 1s-0.1s.

4. How do the expertises of the supervisors complement each other? (≤ 100 words please)

- A.Kornyshev is a leading expert in the theory of electrified interfaces. He has developed theoretical approaches to describe the adsorption behaviour of nanoparticles at electrified interfaces and their optical signal.

- F.Bresme is an expert in the simulations and theory of nanoparticles at interfaces. He has developed algorithms and models to quantify the free energy of adsorption and nanoparticle interactions at atomic and mesoscopic levels.

- A.Horsfield is an expert on Density Functional Theory of solids. He will supervise the computation of the dielectric response of of nanoparticles of different size, shape and composition -- targeted by the theory to reach the demanded mirror effect.

5. Is there a self-contained 12-week MSc project that would usefully initiate this PhD project? (If the answer is no the project will not be offered as an MSc project)

Yes. The 12-week project will be based on Molecular Dynamics simulations of a single nanoparticle (functionalised with ionic groups) at the interface of two immiscible electrolyte solutions. The aim will be to investigate the stability of the particle at the interface as a function of the bias voltage and the nanoparticle charge.