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

1st supervisor
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3rd supervisor (optional)
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Please complete the following:

1. Project title

Using nanowires to smell

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

Checking planes for explosives, monitoring food quality and testing human breath for signs of disease are some of the applications of electronic noses. Existing devices have been optimised to detect particular sets of compounds, but generally lack the ability to be tuned to detect user specified molecules while in operation. This is in striking contrast to the human nose which can respond to endless new chemical species provided only that the molecules are small enough to fit the receptors. We are developing a versatile electronic nose based on the theory of Luca Turin for olfaction in humans ("Could humans recognise odor by phonon assisted tunneling?", Jennifer C. Brookes, F. Hartoutsiou, A. P. Horsfield, and A. M. Stoneham, Phys. Rev. Lett. 98 038101 (2007)) that proposes that receptors respond to the vibrational frequencies of molecules. The proposed device will be constructed from InAs-InP nanowires ("Nanowire resonant tunneling diodes", M. T. Bjork et al, Applied Physics Letters, 81, 4458 (2000)) and can be tuned to respond to a particular type of molecule simply by the application of a bias. Early simulations have demonstrated the feasibility of the

device, and an experimentalist (Paul Warburton, UCL) now has funding to build nanowire devices that he can investigate. In this project you will extend the device simulator to make it more realistic and will carry out state of the art DFT simulations using ONETEP to obtain key parameters of the simulators.

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

The device simulation uses the effective mass approximation to remove atomistic detail and regions up to microns in length. The parameters that feed into these calculations are obtained from density functional theory simulations involving systems of atomic dimensions.

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

Arash Mostofi is an expert in linear scaling DFT, used to obtain the fundamental data. Andrew Horsfield has been using the effective mass approximation for a couple of years now to simulate nanowire devices.

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)

The student could modify the current device simulator to include the scattering off an oscillator to introduce the effect of inelastic scattering. This is an important simulation to obtain the qualitative effect of attached molecules on the conductance of the device.