MAP-fis Essay Proposal, 2013-2014

Supervisor/Co-Supervisor

Name: Rui N. Pereira/Maria Rute Ferreira André

e-mail: rnpereira@ua.pt/rferreira@ua.pt

Title

"Core-shell and core-host interaction effects on the optoelectronic properties of functional silicon-nanoparticles"

Area

Physics of semiconductor nanoparticles

Summary of Proposal

Crystalline silicon nanoparticles (SiNPs) are currently under intense investigation because they combine the unique features of Si at the nanoscale (*e.g.* wavelength tunable light emission and light absorption spectrum,[1] multiple exciton generation,[2] and possibility of doping[3,4]) with the versatile and inexpensive device fabrication associated with nanoparticle processing.[5] These efforts have readily resulted in the practical demonstration of thermoelectrics,[6] solar energy to electricity conversion,[6] and light emission[7,8] with thin films fabricated from SiNPs.

The step from isolated NPs to functional NPs raises novel questions and challenges inherent to NP building blocks, including their sensitivity to the surface shell and surrounding environment. Due to the small dimensions of SiNPs, the large surface shell and species chemically/physically attached to the NP surface will become more important than in bulk dimensions. Thus, interface- and surface-related phenomena will eventually dominate the optical and electronic response. The interaction between the NP core and its surrounding may in fact become a valuable tool for engineering nanometer-scale devices. To maintain a high degree of flexibility for potential applications, it is necessary to tailor and optimize the desired shell and host properties without compromising the useful properties of the NPs. Despite the potential of functional SiNPs for

application in future technologies, major scientific advances are needed before useful technologies become a reality. In this essay we will revise the synthesis, processing and optoelecronic properties of SiNP systems, in which the NPs surface is composed of native oxide shell[2,3,9-12] or organic grups[13]. Particular attention will be given to charge and energy transfer issues.

References

1. Gupta, A., Swihart, M. T. & Wiggers, H. Luminescent Colloidal Dispersion of Silicon Quantum Dots from Microwave Plasma Synthesis: Exploring the Photoluminescence Behavior Across the Visible Spectrum. *Advanced Functional Materials* **19,** 696–703 (2009).
2. Beard, M. C., Knutsen, P. K., Yu P., Luther, J. M., Song, Q., Metzger, W. K., Ellingson, R. J. & Nozik, A.J. Multiple exciton generation in colloidal silicon nanocrystals. *Nano Letters* **7,** 2506–2512 (2007).
3. Stegner, A. R., Pereira, R. N., *et al.* Electronic transport in phosphorus-doped silicon nanocrystal networks. *Physical Review Letters* **100,** 26803 (2008); ***Id.*** Doping efficiency in freestanding silicon nanocrystals from the gas phase: Phosphorus incorporation and defect-induced compensation. *Physical Review B* **80,** 165326 (2009).
4. Pi, X. D., Gresback, R., Liptak, R. W., Campbell, S. A. & Kortshagen, U. Doping efficiency, dopant location and oxidation of Si nanocrystals (vol 92, art no 123102, 2008). *Applied Physics Letters* **92,** 123102 (2008).
5. Mangolini, L. & Kortshagen, U. Plasma-assisted synthesis of silicon nanocrystal inks. *Advanced Materials* **19,** 2513 (2007).
6. Liu, C. Y., Holman, Z. C. & Kortshagen, U. R. Hybrid Solar Cells from P3HT and Silicon Nanocrystals. *Nano Letters* **9,** 449–452 (2009); ***Id.*** Optimization of Si NC/P3HT Hybrid Solar Cells. *Advanced Functional Materials* **20,** 2157–2164 (2010).
7. Cheng, K. Y., Anthony, R., Kortshagen, U. R. & Holmes, R. J. Hybrid Silicon Nanocrystal-Organic Light-Emitting Devices for Infrared Electroluminescence. *Nano Letters* **10,** 1154–1157 (2010); ***Id.*** High-Efficiency Silicon Nanocrystal Light-Emitting Devices; *Nano Letters* **11,** 1952–1956 (2011).
8. Maier-Flaig, F., Rinck, J., Stephan, M., Bocksrocker, T., Bruns, M., Kübel, C., Powell, A. K., Ozin G. A., & Lemmer U. Multicolor silicon light-emitting diodes (SiLEDs). *Nano letters* **13,** 475–80 (2013).
9. Hua, F. J., Swihart, M. T. & Ruckenstein, E. Efficient surface grafting of luminescent silicon quantum dots by photoinitiated hydrosilylation. *Langmuir* **21,** 6054–6062 (2005).
10. Pi, X. D., Mangolini, L., Campbell, S. A. & Kortshagen, U. Room-temperature atmospheric oxidation of Si nanocrystals after HF etching. *Physical Review B* **75,** 85423 (2007).
11. Eyre, R., Goss, J. & Briddon, P. Effect of progressive oxidation on the optical properties of small silicon quantum dots: A computational study. *Physical Review B* **77,** 245407 (2008).
12. Dalpian, G. & Chelikowsky, J. Self-Purification in Semiconductor Nanocrystals. *Physical Review Letters* **96,** 226802 (2006).
13. Reboredo, F. a & Galli, G. Theory of alkyl-terminated silicon quantum dots. *The journal of physical chemistry. B* **109,** 1072–8 (2005).