MINUTES

2nd META Meeting

October 3rd – 4th 2011

held at CNMS, Oak Ridge National Laboratory (US)

Participants WP1

Massimo Celino (MC)	**Centre NAST**
Piero Morales (PM)	**Centre NAST**
Scott Retterer(SR)	**CMNS**
Mike Simonson (MS)	**SNS**
Sean Smith (SS)	**CNMS director**
Bobby Sumpter (BS)	**CMNS**
Sean Smith (SS)	**CMNS**

Participants WP2

Carla Andreani (CA)	**Centre NAST**
Giuseppe Balestrino (GB)	**Centre NAST (in skype conference with NAST Centre)**
Silvia Licoccia (SL)	**Centre NAST Director (in skype conference with NAST Centre)**
Stephen Jesse (SJ)	**CMNS**
Kumar Amit (KA)	**CMNS**
Sergei V. Kalinin (SK)	**CMNS**
Art Baddorf (AB)	**CMNS**

WP1:

MS remains META project reference person for CNMS

PM illustrates progresses on DNA nanogrids assemblage and on peptide adhesion measurements

a) peptides quoted in the literature as specifically adhering onto Cr, TiO2 and ZnO by the phage display technique have been tested in Rome by fluorescence measurements of TAMRA tagged peptides: they show adequate adhesion rate but rather low specificity (factor 2-2.5). However more reliable measurements based on AFM on ultraflat surfaces are necessary, which will be performed in the next weeks.

b) Synthesis and PAGE purification of the component oligonucleotides of DNA grids are now finished and first assemblage attempts of the grids are being performed. So far only 20 nm sided squares made of four "tiles" have been attempted. AFM measurements of such structures adsorbed on cleaved mica show very few assembled square structures embedded in a lot of nanometer sized debris, possibly buffer salts nanocrystals or oligonucleotides clusters. A few long DNA strands have also been observed. Thus the assemblage yield seems much lower than reported in the literature and the proper concentration of the solution, both in terms of oligonucleotides and buffer salts have to be achieved.

MS
suggestions:

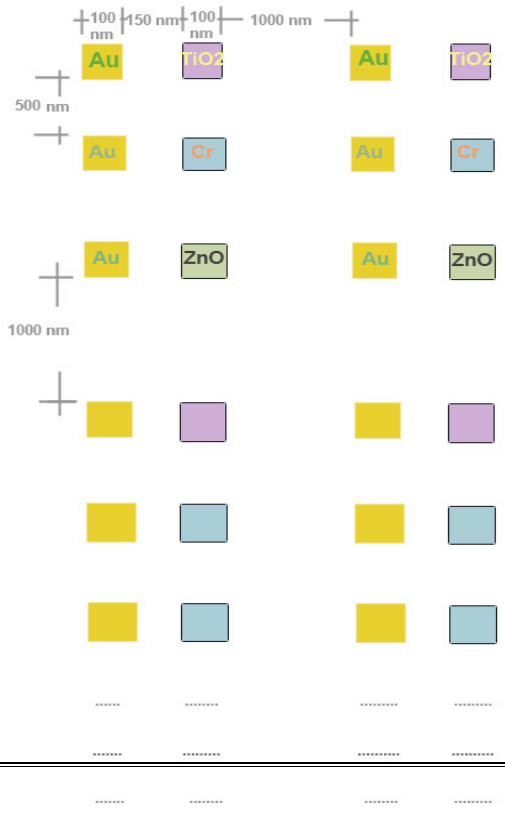
1) Deposit attoliter droplet solution via nanomanipulator and nanoneedle only on fixing pads. Do this under SEM observation, possibly the high pressure, environmental SEM available at CNMS.
PM to check if environmental SEM is operational at Casaccia. First attempts can be made with old Cambridge s200. PM also to check cost and availability of Kleindiek injector system or to check possibility to make injector system using microfactory workshop

2) apply potentials to substrate in attempt to polarize adhesion pads while depositing adhesive peptides by nanoneedle. (depends on lithography for electrical connection to pads, but can be made big for first attempts.

SR responsible for nanofabrication of CNMS

PM illustrates general scheme of project WP1 and needs for improvement of available lithographic nanofabrication technique in order to obtain metal or oxides spots small compared to the 60 nm dimension of the whole DNA grid.
SR suggests:
a) Essential to first go through easy pads fabrication with relaxed requirements.
Can fabricate numerous sets of pads couples:

Gold 100 nm spot – 150 nm spacing – Cr 100 nm spot ** 150 nm is only a typical value*
500 nm free



Gold 100 nm spot – 150 nm spacing –TiO2 100 nm spot
500 nm free
Gold 100 nm spot – 150 nm spacing – ZnO 100 nm spot
1 micron free
Repeated 100 times on substrate to be selected (mica, SiOx, Si nitride) See sketch below.

These spots couples will be used for experiments where the spots will be connected by 200 nm long DNA strands or double strands endowed with specifically sticky peptides at their ends.

CNMS team agrees also to supply patterned metal/oxides surfaces to allow AFM measurement of specific peptides adhesion

To investigate availability and cost of specific peptides tagged on *200 nm DNA strands (Action PM).

b) PhD student Mario Caruso to learn EBL and attempt pushing e-beam lithography performance narrowing progressively sizes and spacing's (March- April 2012)

c) Attempt to fabricate complete system of sets of 4 different pads via EBL +FIB

BS responsible for computational simulation of peptides

MC illustrates the progresses on simulations in Rome. Three peptides simulations have been prepared following indications from the literature:

AMRKLPDAPGMH	adhering on TiO_2
PGMDRQQHQKTEAT	adhering on Cr
RIGHGRQIRKPL	adhering on ZnO

They have been simulated in water by long molecular dynamics simulations to allow them to find the most reliable folding in water.
At the same time several TiO_2 surfaces have been modeled, by using DFT molecular dynamics, to reproduce low Miller index surfaces.

The next step is the simulation of a system composed of the most stable TiO2 surface and of the corresponding peptide, that has been indicated by experiment to be able to adhere on that surface. This system should be simulated in presence of water molecules.
BS and **MC** agree on the observation that accurate calculation of DFT type should be used to better characterize the adhesion of the entire peptide on the surface. However this approach is extremely heavy from the computational side. **MC** and **BS** consider the possibility of simulation of such large system with the accuracy of an ab-initio code. To this aim all the methods and codes available to CNMS has been reviewed and considered for this system. The result of the discussion is that CNSM does not have a computational code that is suitable for this system. **BS** excludes also the use of the NWChem code, improved version of the CNMS group, that has been used in the recent past for simulating a peptide in interaction with a C60 cluster.

In this framework, attempt to use the high performance ORNL computer could be successful. This powerful computer should have enough memory to store all the data of the entire system and enough processors to simulate the system with different starting conditions at the same time. Thus in the next months, Rome in collaboration with ORNL will design several optimized starting configurations and several input for the code Quantum Expresso to run efficiently this system on the ORNL computer. As soon as possible **MC** will submit a request of access to the ORNL computer.

The entire system is composed by 300 TiO_2 atoms, 200 peptide atoms and about 1000 water molecules. It is hard to estimate the memory required at run time: a large number of processors will be used to load in the system memory all the system. Moreover, since there is not a unique way to approach the peptide on the surface , several starting configurations will be built up with the peptide in different orientations.

The other two computational issues of the META project have been briefly discussed: the simulation of the peptide interaction with the DNA molecule and the conductivity properties of the DNA-redox protein systems that will be selfassembled as a goal of the project.
In both cases **BS** at the moment cannot share efforts on either subject. There is no one available at the moment to tackle these issues **BS** suggests to contact Rosa De Felice, who is already collaborating with CNMS, and is an expert for the conductivity properties of these materials.

SS, CNMS director

PM illustrate META project aims with regard to WP2 and WP1
SS agrees on aims and methodologies
Decision to submit user proposals to CNMS board within next deadline on three proposals:

WP1:

a) Nanofabrication (drafted by **PM**)
b) Computational simulation of peptides (drafted by **MC**)

WP2: (drafted by G. Balestrino- S. Licoccia)

Actions: **PM** and **MC** send proposals draft to **MS**, **SR** and **BS**, have their comments, amend proposals and submit to board within deadline, cc to **MS, SR, BS**, **SS** and Project coordinator **SL**

WP2:

Team agrees on several outstanding interrelated issues, including (a) logistics for the visit, (b) CNMS user proposals, and (c) scientific topics to be pursued.

I. Logistics

With respect to logistics (including places to live, travel within
Knoxville-ORNL [e.g. car required], site access to ORNL in case work is supported by user proposal or not) the best person to contact is Art Baddorf (who is the group leader). Note that things will differ somewhat depending on whether there is an active user proposal thought normal channel (which has its own timescale for review), rapid user access project (which typically has very limited scope), or whether the proposal is either unsuccessful, or review times are too large for META plans.

II. Science

With respect to science, **SK** identifies several potential areas for collaboration:

1. For SDC system, we are interested in (a) thickness series for single concentration and (b) for fixed thickness, a composition series (may be from zero to above stability limit - ESM can actually give nice images if the system starts to undergo the decomposition above the miscibility limit). These two

directions are covered by original mail by **GB**, who proposed to look at relaxed *vs.* non-relaxed film.

2. Similarly for SDC film, playing with different substrates can also be interesting to explore the role of ionic and electronic conductivity of substrate and misfit strain on the ionic activity. We may be particularly interested in electronically conductive ionically blocking substrates, but if you feel that there are other series you can make and will be interested in, that will be great.

For these studies, it will be great to know what other characterization methods you plan to apply (ORR activity mapping, etc.).

3. **CA** mentioned our potential interest in H-conductors of the Y doped BZO family and potential use of neutron data to elucidate proton transport mechanisms. We have done some preliminary studies on H-conductors, and the technique definitely works. That said, it is a more complex problem then purely oxygen conductors (two types of ionic carriers). It may be an interesting study as a function of temperature or water partial pressure; we have capabilities to do that (in principle - we have the equipment arrived 2-3 weeks ago, but did not connect it yet). With respect to this system, is it one sample or a composition series, etc?

4. As we discussed, cross-sectioned or beveled interfaces with superionic behavior will be a very interesting object, but sample preparation is the major issue that we are not equipped to address within the group (if you can make these, let us know).

III. Projects

SDC work will form a good basis for CNMS project (the draft that **GB** have sent is an excellent start). For reasons of science and logistics (typical user project is 2 weeks of microscope time), **SK** thinks it makes sense to write at least one additional proposal for H conductors or interfaces (per your interest). Of course, it makes sense to have all sample for the visit!

10th October 2011