# Mikala Grubb - Publications - DTU Orbit (15/01/2016)

## Direct imaging of hexaamine-ruthenium(III) in domain boundaries in monolayers of single-stranded DNA

We describe adsorption and identification of the binding sites of [Ru(NH3)(6)](3+) (RuHex) molecules in a closely packed monolayer of a 13-base ss-DNA on Au(111) electrodes by electrochemical in situ scanning tunneling microscopy (STM), cyclic voltammetry and interfacial capacitance data. In situ STM at single-molecule resolution shows that RuHex adsorbs only at the domain borders and near defects. Together with the electrochemical data that show a negative redox potential shift for RuHex adsorbed to DNA strands, this strongly suggests that RuHex binds only to the exposed phosphate groups in the DNA backbone.

#### General information

State: Published

Organisations: Department of Chemistry, NanoChemistry

Authors: Grubb, M. (Intern), Wackerbarth, H. (Intern), Wengel, J. (Ekstern), Ulstrup, J. (Intern)

Pages: 1410-1413 Publication date: 2007

Main Research Area: Technical/natural sciences

#### **Publication information**

Journal: Langmuir Volume: 23 Issue number: 3 ISSN (Print): 0743-7463

Ratings:

BFI (2015): BFI-level 2 BFI (2014): BFI-level 2

ISI indexed (2013): ISI indexed yes

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BFI (2011): BFI-level 2

ISI indexed (2011): ISI indexed yes

BFI (2010): BFI-level 2 BFI (2009): BFI-level 2 BFI (2008): BFI-level 1 Original language: English

DOIs:

10.1021/la062555z Source: orbit Source-ID: 214814

Publication: Research - peer-review > Journal article - Annual report year: 2007

#### Adsorption of Short DNA and LNA Oligonucleotides on Single-Crystal Au(111)-Electrode Surfaces

#### General information

State: Published

Organisations: Department of Chemistry, Experimental Surface and Nanomaterials Physics, Department of Physics, NanoChemistry, Center for Individual Nanoparticle Functionality, Center for Nanoteknologi, University of Southern Denmark

Authors: Wackerbarth, H. (Intern), Grubb, M. (Intern), Wengel, J. (Ekstern), Chorkendorff, I. (Intern), Ulstrup, J. (Intern)

Pages: L22-L27 Publication date: 2006

Main Research Area: Technical/natural sciences

## **Publication information**

Journal: Surface Science

Volume: 600

ISSN (Print): 0039-6028

Ratings:

BFI (2015): BFI-level 1 BFI (2014): BFI-level 1 ISI indexed (2013): ISI indexed yes

BFI (2013): BFI-level 1 BFI (2012): BFI-level 1

ISI indexed (2012): ISI indexed yes

BFI (2011): BFI-level 1

ISI indexed (2011): ISI indexed yes

BFI (2010): BFI-level 1 BFI (2009): BFI-level 1 BFI (2008): BFI-level 1 Original language: English

Source: orbit Source-ID: 194517

Publication: Research - peer-review > Journal article - Annual report year: 2006

## Identification of Single-Stranded DNA by In Situ Scanning Tunneling Microscopy

#### General information

State: Published

Organisations: Department of Chemistry

Authors: Grubb, M. (Intern), Wackerbarth, H. (Intern), Ulstrup, J. (Intern)

Pages: 7734-7735 Publication date: 2006

Main Research Area: Technical/natural sciences

#### **Publication information**

Journal: American Chemical Society. Journal

Volume: 128

ISSN (Print): 0002-7863

Ratings:

BFI (2015): BFI-level 2 BFI (2014): BFI-level 2

ISI indexed (2013): ISI indexed yes

BFI (2013): BFI-level 2 BFI (2012): BFI-level 2

ISI indexed (2012): ISI indexed yes

BFI (2011): BFI-level 2

ISI indexed (2011): ISI indexed yes

BFI (2010): BFI-level 2 BFI (2009): BFI-level 2 BFI (2008): BFI-level 2 Original language: English

Source: orbit Source-ID: 194476

Publication: Research - peer-review > Journal article - Annual report year: 2006

## Kemi og Bioteknologi på Nanoskala og Enkeltmolekyle Niveau

# **General information**

State: Published

Organisations: Department of Chemistry, Imperial College London, Technical University of Munich

Authors: Jensen, P. S. (Intern), Grubb, M. (Intern), Welinder, A. C. (Intern), Albrecht, T. (Ekstern), Hansen, A. G. (Ekstern)

, Wackerbarth, H. (Ekstern), Zhang, J. (Intern), Chi, Q. (Intern), Ulstrup, J. (Intern)

Pages: 92-104

Publication date: 2006

# Host publication information

Title of host publication: Kemiske Horisonter

Place of publication: DTU
Publisher: Kemisk Institut, DTU
ISBN (Print): 87-91233-07-0

Main Research Area: Technical/natural sciences

Source: orbit Source-ID: 194561

Publication: Education > Book chapter - Annual report year: 2006

#### Electrochemistry and bioelectrochemistry towards the single-molecule level: Theoretical notions and systems

Surface structures controlled at the nanometer and single-molecule levels, with functions crucially determined by interfacial electron transfer (ET) are broadly reported in recent years, with different kinds of electrochemically controlled nanoscale/single molecule systems. One is the broad class of metallic and semiconductor-based nanoparticles, nanoarrays, nanotubes, and nanopits. Others are based on self-assembled molecular monolayers. The latter extend to bioelectrochemical systems with redox metalloproteins and DNA-based molecules as targets. We overview here some recent achievements in areas of interfacial electrochemical ET systems, mapped to the nanoscale and single-molecule levels. Focus is on both experimental and theoretical studies in our group. Systems addressed are organized monolayers of redox active transition metal complexes, and metalloproteins and metalloenzymes on single-crystal Au(111)-electrode surfaces. These systems have been investigated by voltammetry, spectroscopy, microcantilever technology, and scanning probe microscopy. A class of Os-complexes has shown suitable as targets for electrochemical in situ scanning tunnelling microscopy (STM), with close to single-molecule scanning tunnelling spectroscopic (STS) features. Mapping of redox metalloproteins from the three major classes, i.e. blue copper proteins, heme proteins, and iron-sulfur proteins, at the monolayer and single-molecule levels have also been achieved. In situ STM and spectroscopy of redox molecules and biomolecules have been supported by new theoretical frames, which extend established theory of interfacial electrochemical ET. The electrochemical nanoscale and single-molecule systems discussed are compared with other recent nanoscale and single-molecule systems with conspicuous device-like properties, particularly unimolecular rectifiers and single-molecule transistors. Both of these show analogies to electrochemical in situ STM features of redox molecules and biomolecules

#### General information

State: Published

Organisations: Department of Chemistry

Authors: Zhang, J. (Intern), Chi, Q. (Intern), Albrecht, T. (Intern), Kuznetsov, A. (Ekstern), Grubb, M. (Intern), Hansen, A.

(Ekstern), Wackerbarth, H. (Intern), Welinder, A. C. (Intern), Ulstrup, J. (Intern)

Pages: 3143-3159 Publication date: 2005

Main Research Area: Technical/natural sciences

## **Publication information**

Journal: ELECTROCHIMICA ACTA 50

Volume: 50 Sp.Iss. Issue number: 15 ISSN (Print): 0013-4686

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BFI (2015): BFI-level 2 BFI (2014): BFI-level 2

ISI indexed (2013): ISI indexed yes

BFI (2013): BFI-level 1 BFI (2012): BFI-level 1

ISI indexed (2012): ISI indexed yes

BFI (2011): BFI-level 1

ISI indexed (2011): ISI indexed yes

BFI (2010): BFI-level 1 BFI (2009): BFI-level 1 BFI (2008): BFI-level 1 Original language: English

Source: orbit Source-ID: 188076

Publication: Research - peer-review > Journal article - Annual report year: 2005

## Properties and Hybridisation of DNA-Based Molecules towards the Single-Molecule Level"

#### General information

State: Published

Organisations: Department of Chemistry

Authors: Grubb, M. (Intern), Wackerbarth, H. (Intern), Ulstrup, J. (Intern)

Number of pages: 211

Pages: 49-50

Publication date: 2005

#### Host publication information

Title of host publication: NanoTech insight 2005: the International Conference on Nanotechnology: Science and

Applications, February 20-25th 2005, Luxor, Egypt: Book of Abstracts

Publisher: Sabry Corp

Main Research Area: Technical/natural sciences

Conference: International Conference on Nanotechnology, Luxor, Egypt, 20-25 February, 01/01/2005

Source: orbit Source-ID: 188520

Publication: Research > Conference abstract in proceedings – Annual report year: 2005

# Self-Assembly of Biomolecules on Electrode Surfaces; Oligonucleotides, Amino Acids, and Proteins towards the Single-Molecule Level

#### General information

State: Published

Organisations: Department of Chemistry

Authors: Wackerbarth, H. (Intern), Zhang, J. (Intern), Grubb, M. (Intern), Hansen, A. G. (Intern), Ooi, B. L. (Intern),

Christensen, H. E. M. (Intern), Ulstrup, J. (Intern)

Pages: 485-516 Publication date: 2005

## Host publication information

Title of host publication: Electrochemistry of Nucleic Acids and Proteomics: Towards Electrochemical Sensors and

Proteomics

Volume: Chapter 15

Place of publication: Amsterdam

Publisher: Elsevier

Editors: Palecek, E., Scheller, F., Wang, J. Main Research Area: Technical/natural sciences

Source: orbit Source-ID: 188512

Publication: Research - peer-review > Book chapter - Annual report year: 2005

# Electronic Properties and Hybridisation of DNA-Based Molecules towards the Single-Molecule Level.

One page in Book of Abstracts.

# General information

State: Published

Organisations: Department of Chemistry

Authors: Grubb, M. (Intern), Wackerbarth, H. (Intern), Ulstrup, J. (Intern)

Publication date: 2004

Event: Abstract from Workshop on NanoPhysics of DNA, Bad Honnef, Germany, 22nd - 24th March, .

Main Research Area: Technical/natural sciences

Source: orbit Source-ID: 159066

Publication: Research > Conference abstract for conference - Annual report year: 2004

# Highly Ordered Oligonucleotide Domain formation on Au(111),

Book of Abstracts, 4.1.4 - Talk.

#### General information

State: Published

Organisations: Department of Chemistry, Department of Micro- and Nanotechnology

Authors: Wackerbarth, H. (Intern), Grubb, M. (Intern), Marie, R. C. W. (Intern), Boisen, A. (Intern), Ulstrup, J. (Intern)

Publication date: 2004

Event: Abstract from The Eighth World Congress on Biosensors., Granada, Spain, 24-26. May, .

Main Research Area: Technical/natural sciences

Source: orbit Source-ID: 159073

Publication: Research > Conference abstract for conference - Annual report year: 2004

## Interfacial electron transfer at the single molecule level.

## General information

State: Published

Organisations: Department of Chemistry

Authors: Albrecht, T. (Intern), Zhang, J. (Intern), Chi, Q. (Intern), Welinder, A. (Ekstern), Hansen, A. G. (Intern), Jensen, P.

(Ekstern), Grubb, M. (Intern), Wackerbarth, H. (Intern), Ulstrup, J. (Intern)

Publication date: 2004

Event: Paper presented at Imperial College, London, United Kingdom.

Main Research Area: Technical/natural sciences

Source: orbit Source-ID: 178199

Publication: Research > Paper - Annual report year: 2004

### Long-range order of organized oligonucleotide monolayers on Au(111) electrodes

Oligonucleotides modified by a hexamethylene linker group adsorb on gold electrodes via Au-S bond formation. We have obtained novel data for adsorption of thiol-modified (HS) single-strand HS-10A and double-stranded HS-10AT oligonucleotides and for analogous thiol-free 10A (A = adenine) and 10T (T = thymine) nonspecifically adsorbed as reference molecules. Mercaptohexanol has served as a second reference molecule. The data are based on cyclic and differential pulse voltammetry, interfacial capacitance data, and in situ scanning tunneling microscopy (STM) directly in an aqueous buffer solution, with electrochemical potential control of both the sample electrode and the tip. All the data are based on single-crystal, atomically planar Au(111)-electrode surfaces. The high sensitivity of such surfaces provides accurate HS-10A and HS-10AT electrode coverages on the basis of the reductive desorption of the Au-S bond. The coverage is high and in keeping with dense monolayers of adsorbed HS-10A and HS-10AT in an upright or tilted orientation, with the oligonucleotide backbone repelled from the strongly negatively charged electrode surface. Adsorbed thiol-free 10A only gives aAu(111)-reconstruction peak, while 10T shows a subtle pattern involving pronounced voltammetric adsorption peaks indicative of both nonspecific adsorption via single thymine units and potential-dependent structural reorganization in the surface layer. In situ STM supports these findings at the molecular level. In situ STM of HS-10A discloses large, highly ordered domains at strongly negative sample potentials. Reversible domain formation and disordering could, moreover, be controlled by an electrochemical potential variation in the negative and positive directions, respectively. 10A and 10T did not form ordered adsorbate domains, substantiating that domain formation rests on adsorption of thiol-modified oligonucleotide adsorption in an upright or tilted orientation. The comprehensive, highresolution information reported may hold prospects for single-molecule electronic conduction and molecular-scale mapping of oligonucleotide hybridization.

## General information

State: Published

Organisations: Department of Chemistry

Authors: Wackerbarth, H. (Intern), Grubb, M. (Intern), Zhang, J. (Intern), Hansen, A. G. (Intern), Ulstrup, J. (Intern)

Pages: 1647-1655 Publication date: 2004

Main Research Area: Technical/natural sciences

#### **Publication information**

Journal: LANGMUIR

Volume: 20 Issue number: 5 ISSN (Print): 0743-7463

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BFI (2013): BFI-level 2 BFI (2012): BFI-level 2

ISI indexed (2012): ISI indexed yes

BFI (2011): BFI-level 2

ISI indexed (2011): ISI indexed yes

BFI (2010): BFI-level 2 BFI (2009): BFI-level 2 BFI (2008): BFI-level 1 Original language: English

Source: orbit Source-ID: 156010

Publication: Research - peer-review > Journal article - Annual report year: 2004

# Ordered Monolayers of Oligonucleotide-based Molecules on Single-Crystal Au(111) Electrode Surfaces.

One page in Book of Abstracts. Talk.

#### **General information**

State: Published

Organisations: Department of Chemistry

Authors: Wackerbarth, H. (Intern), Grubb, M. (Intern), Wengel, J. (Ekstern), Ulstrup, J. (Intern)

Publication date: 2004

Event: Abstract from Workshop on NanoPhysics of DNA, Bad Honnef, Germany, 22nd - 24th March, .

Main Research Area: Technical/natural sciences

Source: orbit Source-ID: 159068

Publication: Research > Conference abstract for conference - Annual report year: 2004

## Self-Assembly of Sulfur Achored Oligonucleotide.

Book of Abstracts, L2. - Talk.

## **General information**

State: Published

Organisations: Department of Chemistry, Department of Micro- and Nanotechnology

Authors: Wackerbarth, H. (Intern), Grubb, M. (Intern), Marie, R. C. W. (Intern), Boisen, A. (Intern), Ulstrup, J. (Intern)

Publication date: 2004

Event: Abstract from International Conference Electrified Interfaces., Spain, 11-16. July, .

Main Research Area: Technical/natural sciences

Source: orbit Source-ID: 159074

Publication: Research > Conference abstract for conference - Annual report year: 2004

## Single-Stranded Oligonucleotides on Single-Crystal Au(111)-Surfaces

Poster.

# General information

State: Published

Organisations: Department of Chemistry, Department of Systems Biology

Authors: Grubb, M. (Intern), Wackerbarth, H. (Intern), Kristoffersen, P. (Intern), Ulstrup, J. (Intern)

Publication date: 2004

Event: Poster session presented at Ph.D.-Summer School, : Molecular Nanotechnology, KolleKolle, Denmark 16-27.

August, .

Main Research Area: Technical/natural sciences

Source: orbit Source-ID: 159076

## Single-Stranded Oligonucleotides on Single-Crystal Au(111)-Surfaces

Poster and talk.

#### General information

State: Published

Organisations: Department of Chemistry

Authors: Grubb, M. (Intern) Publication date: 2004

Event: Poster session presented at Copenhagen Graduate School of Nanotechnology, University of Copenhagen,

Denmark 20.12.04., .

Main Research Area: Technical/natural sciences

Source: orbit Source-ID: 159077

Publication: Research > Poster - Annual report year: 2004

# Thiol- and Disulfide-modified Oligonucleotide Monolayer Structures on Poloycrystalline and Single-Crystal Au(111) Surfaces

#### **General information**

State: Published

Organisations: Department of Chemistry, Department of Micro- and Nanotechnology, Department of Physics

Authors: Wackerbarth, H. (Intern), Marie, R. C. W. (Intern), Grubb, M. (Intern), Zhang, J. (Intern), Hansen, A. G. (Intern),

Chorkendorff, I. (Intern), Christensen, C. B. V. (Intern), Boisen, A. (Intern), Ulstrup, J. (Intern)

Pages: 474-481 Publication date: 2004

Main Research Area: Technical/natural sciences

## **Publication information**

Journal: Journal of Solid State Electrochemistry

Volume: 8

ISSN (Print): 1432-8488

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ISI indexed (2013): ISI indexed yes

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ISI indexed (2012): ISI indexed yes

BFI (2011): BFI-level 1

ISI indexed (2011): ISI indexed yes

BFI (2010): BFI-level 1 BFI (2009): BFI-level 1 BFI (2008): BFI-level 1 Original language: English

Source: orbit Source-ID: 135933

Publication: Research - peer-review > Journal article - Annual report year: 2004

# Electron transfer behaviour of biological macromolecules towards the single-molecule level

Redox metalloproteins immobilized on metallic surfaces in contact with aqueous biological media are important in many areas of pure and applied sciences. Redox metalloprotein films are currently being addressed by new approaches where biotechnology including modified and synthetic proteins is combined with state-of-the-art physical electrochemistry with emphasis on single-crystal, atomically planar electrode surfaces, in situ scanning tunnelling microscopy (STM) and other surface techniques. These approaches have brought bioelectrochemistry important steps forward towards the nanoscale and single-molecule levels. We discuss here these advances with reference to two specific redox metalloproteins, the blue

single-copper protein Pseudomonas aeruginosa azurin and the single-haem protein Saccharomyces cerevisiae yeast cytochrome c, and a short oligonucleotide. Both proteins can be immobilized on Au(111) by chemisorption via exposed sulfur-containing residues. Voltammetric, interfacial capacitance, x-ray photoelectron spectroscopy and microcantilever sensor data, together with in situ STM with single-molecule resolution, all point to a coherent view of monolayer organization with protein electron transfer (ET) function retained. In situ STM can also address the microscopic mechanisms for electron tunnelling through the biomolecules and offers novel notions such as coherent multi-ET between the substrate and tip via the molecular redox levels. This differs in important respects from electrochemical ET at a single metal/electrolyte interface. Similar data for a short oligonucleotide immobilized on Au(111) show that oligonucleotides can be characterized with comparable detail, with novel perspectives for addressing DNA electronic conduction mechanisms and for biological screening towards the single-molecule level.

## **General information**

State: Published

Organisations: Department of Chemistry, Department of Micro- and Nanotechnology

Authors: Zhang, J. (Intern), Grubb, M. (Intern), Hansen, A. G. (Intern), Kuznetsov, A. (Ekstern), Boisen, A. (Intern),

Wackerbarth, H. (Intern), Ulstrup, J. (Intern)

Pages: S1873-S1890 Publication date: 2003

Main Research Area: Technical/natural sciences

# **Publication information**

Journal: Journal of physics-condensed matter

Volume: 15 Issue number: 18 ISSN (Print): 0953-8984

Ratings:

BFI (2015): BFI-level 1 BFI (2014): BFI-level 1

ISI indexed (2013): ISI indexed yes

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ISI indexed (2012): ISI indexed yes

BFI (2011): BFI-level 1

ISI indexed (2011): ISI indexed yes

BFI (2010): BFI-level 1 BFI (2009): BFI-level 1 BFI (2008): BFI-level 1 Original language: English

Source: orbit Source-ID: 22959

Publication: Research - peer-review > Journal article - Annual report year: 2003