

Center for Nanophase Materials Sciences

2012 User Meeting

Poster Session

Thursday, September 13, 2012
4:00 – 5:00p

Posters will also be available for viewing on Friday, September 14

01

Pillar arrayed chips for planar separation and detection

Teresa Kirchner,¹ Nichole Crane,¹ Chris Freye,² Nickolay Lavrik,² Michael Sepaniak¹

¹Department of Chemistry, University of Tennessee, Knoxville, 552 Buehler Hall 1420 Circle Dr , Knoxville TN 37996

²Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN, 37831

02

Silicon nanopillars for field enhanced surface spectroscopy

Jennifer Charlton,¹ Sabrina Wells,¹ Michael Kandziolka,¹ Igor Merkulov,² Ivan Kravchenko,² Nickolay Lavrik,² James Bradshaw,³ and Michael Sepaniak¹

¹Department of Chemistry, University of Tennessee, Knoxville, 552 Buehler Hall 1420 Circle Dr , Knoxville TN 37996

²Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN, 37831

³Y-12 National Security Complex

03

Extraordinary optical transmission of multimode quantum correlations via localized surface plasmons

Benjamin Lawrie, Philip Evans, Raphael Pooser

Computational Sciences and Engineering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831

04

Nanophotonics: From novel fabrication technologies to reconfigurable photonics

Shuren Hu,¹ Judson D. Ryckman,² Yang Jiao,² Jeremy W. Mares,² and Sharon M. Weiss^{1,2}

¹Department of Physics and Astronomy, Vanderbilt University, Nashville, Tennessee 37235

²Department of Electrical Engineering and Computer Science, Vanderbilt University, Nashville, Tennessee 37235

05

Raman Plasmonic Enhancement based on Biomimetic Metal Nanostructures

Héctor I. Areizaga,¹ Raymond A. Velez-Calder,¹ Marco A. De Jesús,¹ Michael J. Sepaniak,² Nickolay V. Lavrik,³ Ivan I. Kravchenko³

¹Department of Chemistry, University of Puerto Rico, Mayagüez, P.O. Box 9000, Mayagüez, PR 00681

²Department of Chemistry, University of Tennessee, Knoxville, 552 Buehler Hall 1420 Circle Dr , Knoxville TN 37996

³Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN, 37831

06

Single-molecule mobility in confined and crowded femtoliter chambers

C. Patrick Collier

Center for Nanophase Materials Science, Oak Ridge National Laboratory

07

Directed selfassembly of soft matter nanostructures on inorganic surfaces

S. Vespucci,² S. Rettner,¹ S. Baschieri,³ C. Cantale,³ M. Caruso,² C. Dalmastrì,³ C. Lico,³ L. Mosiello,³ P. Morales³

¹Center for Nanoscale Materials Science, Oak Ridge National Laboratory, Oak Ridge, Tennessee

²The NAST Center, Tor Vergata University Unit Viale della Ricerca Scientifica 1, 00136 Roma, Italy

³ENEA, Centro Ricerche Casaccia and NAST Center Via Anguillarese 301 00123 Roma, Italy

08

Bio-inspired Assembly of Silica at the Nanoscale

Juan Pablo Hinestrosa,¹ Jonathan E. Sutton,² David P. Allison,^{3,4} Mitchel J. Doktycz¹,³ Jamie M. Messman,¹ Scott T. Retterer,^{1,3}

¹Center for Nanophase Material Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831

²Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, DE 19716

³Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831

⁴Department of Biochemistry & Cellular & Molecular Biology, University of Tennessee, Knoxville, TN 37996

09

Fracture Strength of Small Diameter Fibers with FIB and Nano-Tensile Testing

M. Kant and D. Penumadu

Civil and Environmental Engineering, University of Tennessee, Knoxville, TN USA

10

A triple beam microscope: Focused laser processing in a scanning ion/electron microscope

N. A. Roberts,^{1,2} G. A. Magel,¹ C. D. Hartfield,¹ T. M. Moore,¹ J. D. Fowlkes³ and P. D. Rack^{2,3}

¹Omniprobe, Inc., an Oxford Instruments Company, 10410 Miller Rd., Dallas, Texas 75238

²Department of Materials Science and Engineering, University of Tennessee, Knoxville, Tennessee 37996

³Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831

11

Characterization of phase-separated, self-assembled, epitaxial Cu₂O-TiO₂ nano-pillar arrays for advanced photovoltaics

Daniela F. Bogorin,¹ Tolga Aytug,¹ Andrew R. Lupini,¹ Sergei Kalinin,¹ Evgheni Strelcov,¹ Ivan I. Kravchenko,¹ Adam J. Rondinone,¹ Ilia N. Ivanov,¹ Victor Maroni²

¹Oak Ridge National Laboratory, Oak Ridge, TN 37831

²Argonne National Laboratory, Argonne IL 60439

12

***Ab initio* based multi-scale modeling of segregation in solids**

Hyunwook Kwak,¹ Yun-kyung Shin,² Adri C. T. van Duin,² and Alex V. Vasenkov¹

¹CFD Research Corporation, 215 Wynn Drive, Huntsville, AL 35805

²Pennsylvania State University, University Park, PA 16802

13

Phosphorous pentasulfide as a novel additive for high-performance lithium-sulfur batteries

Zhan Lin,¹ Zengcai Liu,² Wujun Fu,² Nancy J. Dudney,¹ and Chengdu Liang,^{2*}

¹Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831

²Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831

14

Cr, N, -Codoped TiO₂ Mesoporous Microspheres for Li-ion Rechargeable Batteries

Zhonghe Bi,¹ Craig A. Bridges,¹ Bingkun Guo,¹ Xiao-Guang Sun,¹ Raymond R. Unocic,¹ Harry M Meyer III,² Sheng Dai,¹ and M. Parans Paranthaman¹

¹Chemical Science Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831

²Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831

15

TiO₂ Nanotube Arrays on Porous Ti Foam for Rechargeable Lithium and Sodium Ion Batteries

M. Parans Paranthaman,¹ Zhonghe Bi,¹ Paul A. Menchhofer,² Ryan R. Dehoff,² Craig A. Bridges,¹ Miaofang Chi,² Bingkun Guo,¹ Xiao-Guang Sun,¹ Sheng Dai¹

¹Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831

²Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831

16 Graphitic Mesoporous Carbons as the Supports of Promoted Rhodium and Molybdenum Carbide Catalysts for Alcohol Production from Synthesis Gas

Song-Hai Chai,¹ Jane Y. Howe,² Viviane Schwartz,³ Michelle Kidder,¹ Steven H. Overbury,^{1,3} Sheng Dai,^{1,3,4} De-en Jiang¹

¹Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831

²Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831

³Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831

⁴Department of Chemistry, University of Tennessee, Knoxville, TN 37966

17 Zeolite LTA-Polyimide Nanocomposite Membranes for Natural Gas Separations

Megan Lydon,¹ Kinga Unocic,² Christopher Jones,^{2,3} Sankar Nair,³

¹School of Chemistry & Biochemistry, Georgia Institute of Technology, Atlanta, GA

²Oak Ridge National Laboratory, Oak Ridge, TN

³School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

18 Are the Surfaces of Oxide Nanocrystals With Defined Facets as Perfect as They Appear? – A Case Study of Nanoshaped Ceria Catalysts

Zili Wu, Meijun Li, Steven H. Overbury

Chemical Science Division and Center for Nanophase Materials Sciences

18 Solution-Based Lithium Incorporation and Delamination of Magnesium Diboride

Daniel R. Sexton, Matthew T. Davidson, Christopher A. Barrett and Tina T. Salguero

Department of Chemistry, University of Georgia, Athens, Georgia 30602, USA

20 In situ synthesis of oxynitrides

Craig Bridges

Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee

21 Synthesis of Cadmium Selenide (CdSe) Quantum Dots via an Aerosol Route

He Jing and Da-Ren Chen

Washington University in St. Louis, One Brookings Drive, St. Louis, Missouri, 63130

22 SAXS studies of alkyl chain, temperature, and confinement effects on the structure of room temperature ionic liquids

José Leo Bañuelos,¹ Song Li,² Guang Feng,² Pasquale F. Fulvio,¹ Nikolas Arend,³ Gernot Rother,¹ Antonio Faraone,⁴ Lawrence M. Anovitz,² Patrick Hillesheim,¹ Jianchang Guo,¹ Robert W. Shaw,¹ Sheng Dai,¹ Peter T. Cummings,^{2,5} David J. Wesolowski¹

¹Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee

²Department of Chemical and Biomolecular Engineering, Vanderbilt University, Nashville, Tennessee

³Jülich Center for Neutron Science at the Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, Tennessee

⁴NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland

⁵Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee

23 Enhanced Dispersion and Stability of Platinum on SiO₂ by Surface Modification with ZrO₂ and TiO₂ – Impact on CO Oxidation Performance

Mi-Young Kim,¹ Jae-Soon Choi,¹ Todd J. Toops,¹ Viviane Schwartz,¹ Jihua Chen,¹ Eun-Suk Jeong,² Sang-Wook Han¹

¹Center for Nanophase Materials Science, Oak Ridge National Laboratory

²Chonbuk National University, South Korea

24

Effect of Solvent Quality on the Chain Conformation of Poly(3-Hexylthiophene) (P3HT) in Solution and the Crystalline Morphology of Solution-Casted Thin Film

Jong Kahk Keum,^{1*} Kai Xiao,² Ilia N. Ivanov,² Kunlun Hong,² James F. Browning,^{1*} Gregory S. Smith,¹ Ming Shao,² Kenneth C. Littrell,¹ Adam J. Rondinone,² Andrew E. Payzant²

¹Neutron Scattering Science Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

²Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

25

End Functionalized Conjugated Polymers for Potential Self Assembly and Optoelectronic Applications

T. David,¹ S. Sun,¹ D. Pickel,² and K. Hong²

¹Center for Materials Science (CMR), Norfolk State University

²Center for Nanophase Materials Science, Oak Ridge National Laboratory

26

Charge regulation and local dielectric function in planar polyelectrolyte brushes

Rajeev Kumar¹, Bobby G. Sumpter² and S. Michael Kilbey II^{2,3}

¹ National Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, TN-37831

² Center for Nanophase Materials Science, Oak Ridge National Laboratory, Oak Ridge, TN-37831

³ Department of Chemistry, University of Tennessee, Knoxville, TN-37996

27

Temperature Gradient Interaction Chromatography: An inside look at polymer heterogeneity

Deanna L. Pickel, George C. Morar, David W. Uhrig, S. Michael Kilbey, II

Center for Nanophase Materials Science, Oak Ridge National Laboratory

28

Ab-initio calculations and molecular dynamics simulations of peptide adsorption onto metal oxide surfaces

C. Arcangeli,^{1,2} I. Borriello,^{1,2} M. Celino,^{1,2} M. V. Falessi,¹ P. Morales,^{1,3} N. Pellicciotta,¹ B. G. Sumpter,⁴

¹NAST Centre, Nanoscience & Nanotechnology & Innovative Instrumentation, Università degli Studi di Tor Vergata, Via della Ricerca Scientifica, 1 I-00133 Roma, Italy

²ENEA, UTTMAT-DIAG, Casaccia Research Center, Via Anguillarese 301, I-00123 Roma Italy

³ENEA, UTTMAT-SUP, Casaccia Research Center, Via Anguillarese 301, I-00123 Roma Italy

⁴Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN USA

29

Applications of Scanning Probe Microscopy in Biology

V. Reukov,¹ A.S. Shaporev,¹ G.L. Thompson,² M. Nikiforov,³ S. Jesse,⁴ S. Kalinin,⁴ A. Vertegel¹

¹Clemson University, Department of Bioengineering, Clemson, SC

²Air Force Research Laboratory, San Antonio, TX

³Argonne National Laboratory, Chicago, IL

⁴Center for Nanophase Materials Science, Oak Ridge National Laboratory, Oak Ridge, TN

30

A search model for topological insulators with high-throughput robustness descriptors

Kesong Yang,¹ Wahyu Setyawan,² Shidong Wang,¹ Marco Buongiorno Nardelli,^{3,4} and Stefano Curtarolo,^{1,3,4}

¹Department of Mechanical Engineering and Materials Science, Duke University, Durham, North Carolina 27708

²Pacific Northwest National Laboratory, P.O. Box 999, Richland, Washington 99352

³Department of Physics and Department of Chemistry, University of North Texas, Denton, TX 76203

⁴Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831

⁵Department of Physics, Duke University, Durham, North Carolina 27708

31 On The Information Content of Conductance Histograms: Transport Mechanisms, Cooperative Effects, and Junction Symmetries

Patrick D. Williams,^{1,2} and Matthew G. Reuter^{2,3}

¹Oak Ridge High School, Oak Ridge, TN 37830

²Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831

³Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831

32 Electrochemical Nanowriting on CeO₂ Thin Films

Nan Yang,^{1,3} Sandra Doria,² Amit Kumar,³ Antonello Tebano,¹ Silvia Licoccia,³ Sergei Kalinin,⁴ and Giuseppe Balestrino¹

¹INFM-CNR SPIN and Department of Informatica Sistemi e Produzione, University of Rome, Tor Vergata, Via del Politecnico, 00133, Rome, Italy

²Departement of Physics, University of Rome, La Sapienza, Piazzale Aldo Moro 5, 00185, Rome, Italy

³Department of Chemical Science and Technologies & NAST Center, University of Rome, Tor Vergata, Via della Ricerca Scientifica, 00133, Rome, Italy

⁴Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831

33 Search for new materials - a computational approach

P. Ganesh

Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831

34 Epitaxial growth of highly conductive IrO₂ thin films by pulsed laser deposition

Liang Qiao and Michael D. Biegalski

Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

35 Femtosecond Laser Micro-/Nano-machining of Holes and Lines in Fused Silica

B. K. Canfield, L. Costa, D. Rajput, A. Terekhov, W. H. Hofmeister, and L. M. Davis

Center for Laser Applications, University of Tennessee Space Institute, 411 B. H. Goethert Pkwy, MS 35, Tullahoma, TN 37388

36 The Role of Hydrogen During Si Nanowire Growth

Naechul Shin and Michael. A. Filler

Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

37 Phonon Engineering of Si Nanowires by Controlled Chemical Doping

M.Babaeian,¹ M. Ontl,² T. Jayasekera,¹ A. Calzolari,³ M. B. Nardelli^{4,5}

¹Department of Physics, Southern Illinois University, Carbondale, IL

²South Western Illinois College, REU Participant at Southern Illinois University, Carbondale, IL

³Theory@Elettra Group, DEMOCRITOS National Simulation Center CNR-IOM Istituto Officina dei Materiali, I-34014 Trieste, Italy

⁴Department of Physics and Department of Chemistry, University of North Texas, Denton, Texas 76203

⁵Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831

38 Resonant Infrared Matrix-Assisted Pulsed Laser Evaporation of P3HT-based Bulk Heterojunctions: Small-Angle X-ray Scattering and Photovoltaic Device Characterization

Adrienne D. Stiff-Roberts and Ryan D. McCormick

Duke University, Department of Electrical and Computer Engineering, Box 90291 Durham, NC 27708

39 Novel Fullerene Acceptor Materials for Application in Advanced Organic Photovoltaics

Youjun He, Ming Shao, Kai Xiao, Sean C. Smith, Kunlun Hong

Center for Nanophase Material Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831