William R. Wiley

EMSL

Environmental Molecular Sciences Laboratory

2004 Annual Report

A NATIONAL USER FACILITY FOR THE SCIENTIFIC COMMUNITY

Providing World-Class Research Capabilities for Enabling Fundamental Research on Physical, Chemical, and Biological Processes

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Environmental Molecular Sciences Laboratory 2004 Annual Report

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Contents

Acronyms

AAAS	American Association for the Advancement of Science
ACAP	amphipathic, cationic, antimicrobial peptides
ACS	American Chemical Society
ADAM	A desintegrin and metalloprotease
AES	auger electron spectroscopy
AFM	atomic force microscope (or microscopy)
AFS	Andrew File System
AMT	accurate mass and time (tag)
API	application program interface
ASW	amorphous solid water
AVS	American Vacuum Society
BESAC	Basic Energy Sciences Advisory Committee
BET	Brunauer, Emmett, Teller (method)
BLAST	Basic Local Alignment Search Tool
BOE	buffered oxide etch
CaNS	Computing and Networking Services
CARS	coherent anti-Stokes Raman scattering
CATs	Collaborative Access Teams
CBD	β-catenin destruction
CBED	convergent beam electron diffraction
CCD	charge-coupled device
CCI	Community College Institute
CCN	cloud condensation nuclei
CD	circular dichroism
CE	capillary electrophoretic
CHC	chlorinated hydrocarbon
CIEF	capillary isoelectric focusing
CNE	collaborative network enclave
CPCS	Chemistry & Physics of Complex Systems (Facility)
CPMAS	cross-polarization magic angle spinning
CPMD	Car-Parrinello molecular dynamics
CRIF	Chemistry Research Instrumentation and Facility
CSF	cerebral spinal fluid
CUO	carbon-uranium-oxide
CWC	condensed water content
DFT	density functional theory
DIRB	dissimilatory Fe(III)-reducing bacterium
DMRB	dissimilatory metal-reducing bacteria
DMS	diluted magnetic semiconductor
DNA	deoxyribonucleic acid
DNAPLS	dense nonaqueous phase liquids

DOE	U.S. Department of Energy
DRAM	dynamic random access memory
DREAMS	dynamic range enhancement applied to mass spectrometry
ECM	extracellular matrix
EECS	Electrical Engineering and Computer Science
EELS	electron energy-loss spectroscopy
EGR	epidermal growth factor
EGFR	epidermal growth factor receptor
EMSL	W.R. Wiley Environmental Molecular Sciences Laboratory
EPR	electron paramagnetic resonance
ERDA	elastic recoil detection analysis
ERS	EMSL Resource System
ESD	electron-stimulated desorption
ESEM	environmental scanning electron microscope
ESHQ	EMSL Support and Help Queue (request system)
ESI	electron spectroscopic imaging (as used on page 2-5-4, INSF)
ESI	electrospray ionization
EUS	EMSL User System
EXAFS	extended x-ray absorption fine structure
FAC	frustrated auger configuration
FAU	faujasite
FEM	frequency-domain finite element method
FESEM	field emission scanning electron microscope
FIB	focused ion beam
FLC	Federal Laboratory Consortium
FLIM	fluorescence lifetime imaging microscopy
FPGA	field-programmable gate arrays
FRAM	ferroelectric random access memory
FRET	fluorescence resonance energy transfer
FSAM	fluorinated self-assembled monolayer
FT	Fourier transform
FTICR	Fourier transform ion cyclotron resonance
FTIR	Fourier transform, infrared
FY	fiscal year
GADDS	Geophysical Archive Data Delivery System
GADU	Genome Analysis and Databases Update
GAP	GTPase-activating protein
GDNF	Glial-cell-derived neurotrophic factor
GFP	green fluorescence protein
GIXRD	grazing-incidence x-ray diffraction
GO	gene ontology
GPIB	general purpose interface bus
GR	green rust
GRP78	glucose-regulated protein 78 kDa

GTP	guanosine triphosphate
GVL	Graphics and Visualization Laboratory
HAP	hydroxyapatite
HCV	hepatitis C virus
HDGF	hepatoma-derived growth factor
HE	high-energy
HF	Hartree-Fock (theory)
HFMRF	High Field Magnetic Resonance Facility
high-T_c	high-Curie-temperature
HMEC	human mammary epithelial cells
HP	Hewlett Packard
HPLC	high-performance liquid chromatography
HPMSF	High-Performance Mass Spectrometry Facility
HRM	hydrogen-rich materials
HRTEM	high-resolution transmission electron microscopy
HREELS	high-resolution electron energy loss spectroscopy
HRXRD	high-resolution x-ray diffraction
HSQC	heteronuclear single quantum correlation
I&NS	Interfacial & Nanoscale Science
I&NSF	Interfacial & Nanoscale Science Facility
ICART2	International Consortium for Atmospheric Research on Transport and Transportation
ICAT	isotope-coded affinity tagging
IC&E	Interfacial Chemistry and Engineering
ICR	ion cyclotron resonance
ID	identification
IDF	Integrated Disposal Facility
IDL	Instrument Development Laboratory
IEEE	Institute of Electrical and Electronics Engineers
ILAW	immobilized low-activity waste
IMAC	immobilized metal affinity chromatography
INL	Idaho National Laboratory
IP	Internet Protocol
IPI	International Protein Index
IR	infrared
ITMS	ion-trap mass spectrometry
KDP	archerite (also $KH_2 PO_4$ or potassium dihydrogen phosphate)
LBNL	Lawrence Berkeley National Laboratory
LC	liquid chromatography
LD	laser diode
LDA+U	local density approximation plus a Hubbard U term
LD-ITMS	laser-desorption, ion-trap mass spectrometer
LE	low-energy

LED	light-emitting diode
LEED	low-energy electron diffraction
LET	linear-energy-transfer
MALDI	matrix-assisted laser desorption/ionization
MAS	magic angle spinning
MBE	molecular beam epitaxy
MEC	Minnesota effective core
ML	monolayer
MLWF	maximally localized Wannier function
MMF	Multiscale Modeling Framework
MOCVD	metal organic chemical vapor deposition
MQW	multiple quantum well
MS	mass spectrometry or spectrometer
MSCF	Molecular Science Computing Facility
MS/MS	tandem mass spectrometry
NADPH	nicotinamide adenine dinucleotide phosphate hydrogen
NAPL	nonaqueous phase liquid
NBED	nanometer beam electron diffraction
NC	non-contact
NEAX	Northeast Aerosol Experiment
NESG	Northeast Structural Genomics Consortium
NIH	National Institutes of Health
NIQ	non-isotopic labeling quantification
NMR	nuclear magnetic resonance
NOE	nuclear Overhauser effect
NOESY	nuclear Overhauser effect spectroscopy
NO_x	nitrous oxide
NRA	nuclear reaction analysis
NUC	natural, uranyl-bearing calcite
NWChem	Northwest Computational Chemistry
OPA-MBE	oxygen plasma assisted-molecular beam epitaxy
ORF	open reading frame
PAH	polycyclic aromatic hydrocarbon
PAL	Programmable Array Logic
PAMAM	polyamidoamine
PC	phosphatidylcholine
PDB	Protein Data Bank
PEEM	photo-emission electron microscope
PEELS	parallel electron energy loss spectrometer
PETSc	Portable Extensible Toolkit for Scientific computation
PG	phosphatidylglycerol
PHI	Physical Electronics Instruments
PIXE	proton-induced x-ray emission

PKA	protein kinase A
PMA	4β-phorbol 12-myristate 13-acetate
PMAP	plasma membrane-associated proteins
PN	peroxynitrite
PNC-CAT	Pacific Northwest Consortium-Collaborative Access Team
PNNL	Pacific Northwest National Laboratory
PNWAVS	Pacific Northwest Chapter of the American Vacuum Society
ppb	parts per billion
ppm	parts per million
PR_3	proteinase 3
PSI	Protein Structure Initiative
PSPW	psuedopotential plane-wave
PTR	proton transfer reaction
PWPP-DFT	plane-wave pseudopotential density-functional theory
QCET	Quantitative Cysteinyl-Peptide Enrichment Technology
QCPMG	Quadrupolar Carr-Purcell-Meiboom-Gill (MAS)
QMS	quadrupole mass spectrometer
QTOF	quadrupole time-of-flight
RBS/C	Rutherford backscattering spectrometry/channeling
RDC	residual dipolar coupling
RDF	radial distribution function
REDOR	rotational-echo, double-resonance (NMR)
REV	representative elementary volume
RH	relative humidity
RING	Really Interesting New Gene
RF	radio frequency
RGL	Rosato-Guillope Legrand
RHEED	reflection high-energy electron diffraction
RNA	ribonucleic acid
RNP	ribonucleoprotein
RPLC	reverse-phase liquid chromatography
RPCLC	reverse-phase capillary liquid chromatography
RT	reverse transcription
RTK	receptor tyrosine kinase
Ru-G4OH PAMAM	Ruthenium nanoparticle encapsulated within a hydroxyl-terminated fourth generation poly(amido) amine dendrimer
SAC	Science Advisory Committee
SAC	System Assessment Capability (as used on page 3-1-7)
SAGE	serial analysis of gene expression
SAM	self-assembled monolayer
SAS	surface analysis system (as used on page 2-5-4)
SAS	scanning auger spectrometer
SCF-NDDO	self-consistent-field neglect of diatomic differential overlap
SCX	strong cation exchange

SEM	scanning electron microscopy
SESDAD	surface electronic spectra detected by atomic desorption
SIC	self-interaction correction
SID	surface-induced dissociation
SIMS	secondary ion mass spectrometry
SMART	Simple Modular Architecture Research Tool (genome database)
SMP	symmetrical multiprocessing
SOFC	solid oxide fuel cells
SOM	soil organic matter
SORICID	sustained off-resonance irradiation
SPARC	secreted protein, acidic, cysteine-rich
ss	solid-state
ssh	SecureShell
ssNMR	solid-state nuclear magnetic resonance
SFTEL	Subsurface Flow & Transport Experimental Laboratory
STIM	scanning transmission ion microscopy
STM	scanning tunneling microscopy
STO	strontium titanate
STOMP	Subsurface Transport Over Multiple Phases
STORM	Subsurface Transport Over Reactive Multiple Phases
SWCNT	single-wall carbon nanotube
TACE	TNα converting enzyme
TALOS	Torsion Angle Likelihood Obtained from Shift (and sequence similarity)
TAXRD	triple-axis, x-ray diffraction
TCA	trichloroacetic acid
TCP/IP	transmission control protocol/internet protocol
TDDFT	time-dependent density functional theory
TEAS	Trademark Electronic Application System
TEM	transmission electron microscopy
TGF-α	transforming growth factor-alpha
TMA	trimethylacetate
TMAA	trimethyl acetic acid
TMD	transmembrane domain
TMHMM	transmembrane helices Markov model
TMPP	trimethoxyphenyl phosphonium
TNF-α	tumor necrosis factor-alpha
TOF-SIMS	time-of-flight secondary ion mass spectrometer
TpA	two-photon absorption
TPD	temperature-programmed desorption
TRLFISM	time-resolved fluorescence image
TRLFS	time-resolved laser-induced fluorescence spectroscopy
TSTpA	two-step two-photon absorption
TTA	thionyltrifluoroacetoacetonate

UA	University of Alabama
UAC	User Advisory Committee
UCL	up-conversion luminescence
UHV	ultra-high vacuum
UM	University of Maryland (School of Medicine)
UPS	ultraviolet photoemission
USO	User Services & Outreach
VNMR	Varian nuclear magnetic resonance (software program)
VOC	volatile organic compound
VPN	Virtual Private Network
VRAD	velocity-resolved atomic desorption
WSU	Washington State University
YSZ	yttria-stabilized zirconia
XAFS	x-ray absorption fine structure
XANES	x-ray absorption near-edge structure
XPS	x-ray photoelectron spectroscopy
XRD	x-ray diffraction
XRPD	x-ray powder diffraction
XRR	x-ray reflectivity