



*William R. Wiley*

**EMSL**

Environmental Molecular Sciences Laboratory

**2003 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



# **Environmental Molecular Sciences Laboratory 2003 Annual Report**

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## Acronyms

AAS	atomic absorption spectrophotometry
ACAP	amphipathic, cationic, antimicrobial peptides
ADC	analog digital converter
AES	Auger electron spectroscopy
AFM	atomic force microscopy
AFS	Andrew File System
ALS	advanced light source
APS	American Physical Society
ASW	amorphous solid water
ATR	attenuated total reflectance
BER	base excision repair
BESAC	Basic Energy Sciences Advisory Committee
BLAST	Basic Local Alignment Search Tool
CaNS	Computer and Network Services
CARS	coherent anti-Stokes Raman scattering
CART	classification and regression tree
CATS	Collaborative Access Teams
CBED	convergent beam electron diffraction
CBS	complete basis set
CCD	charge coupled device
CCR	closed-cycle refrigeration
CE	capillary electrophoretic
CHAPS	3-[(3-chloamidopropyl) dimethylammonio]-1-propane sulfonate
CHC	chlorinated hydrocarbon
CID	collision-induced dissociation
CIEF	capillary isoelectric focusing
CP	cross-polarization
CPCS	Chemistry & Physics of Complex Systems
CPD	cyclobutane pyrimidine
CPMAS	cross-polarization, magic-angle-spinning
CPMG	Carr, Purcell, Meiboom, and Gill
CSTR	continuous stirred tank reactor
CTI	constant time imaging
DAGK	prokaryotic diacylglycerolkinase
DBBP	di-butyl-butyl phosphonate
DFT	density functional theory
DI	Digital Instrument
DI/DS	direct-impact, defect-stimulated
DIRB	Dissimilatory Fe(III)-Reducing Bacterium
DLO	diffusion-limited oxidation
DMRB	dissimilatory metal-reducing bacteria

DMS	diluted magnetic semiconductor
DNA	deoxyribonucleic acid
DOE	U.S. Department of Energy
DREAMS	Dynamic Range Enhancement Applied to Mass Spectrometry
DRIFTS	diffuse reflectance
Ecce	Extensible Computational Chemistry Environment
ECL	Experimental Computing Laboratory
EDS	energy dispersive spectroscopy
EDT	2-ethanedithiol
EELS	electron energy-loss spectroscopy
EGFR	epidermal growth factor receptor
ELISA	enzyme-linked immunosorbent assay
EMSL	W.R. Wiley Environmental Molecular Sciences Laboratory
EMSP	Environmental Management Science Program
EPR	electron paramagnetic resonance
EPU	elliptically polarized undulator
ERDA	elastic-recoil detection analysis
ERS	EMSL Resource System
ES&B	Environmental Spectroscopy & Biogeochemistry
ESD	electron-stimulated desorption
ESEM	environmental scanning electron microscope
ESHQ	EMSL Support and Help Queue system
ESI	electron spectroscopic imaging (as used on page 2-5-4)
ESI	electrospray ionization (as used on page 2-4-2)
ESP	electrostatic potential
ET	electron transfer
EUS	EMSL User System
EVA	Enterprise Virtual Array
EXFAS	x-ray absorption fine-structure spectroscopy
FAQs	frequently asked questions
FESEM	field emission scanning electron microscope
FIB	focused ion beam
FPGA	field-programmable gate arrays
FRET	fluorescence resonance energy transfer
FSAM	fluorinated self-assembled monolayer
FT	Fourier transform
FTICR	Fourier transform ion cyclotron resonance
FTIR	Fourier transform, infrared
FTMS	Fourier Transform Ion Cyclotron Resonance Mass Spectrometer
FTS	Fourier transform spectrometer
FWHM	full width at half maximum
FY	fiscal year



GA	Global Arrays
GaN	gallium nitride
GAC	granular activated carbon
GADU	Genome Analysis and Databases Update
GC	gas chromatograph
GFP	green fluorescence protein
GGA	generalized-gradient-approximation
GI	grazing incidence
GIF	Gatan image filter
GIXRD	grazing-incidence x-ray diffraction
GR	green rust
GVL	Graphics and Visualization Laboratory
HA	High Availability
HCN	triple resonance probe with proton ( $^1\text{H}$ ) on the observe coil and a double-tuned second coil for $^{13}\text{C}$ and $^{15}\text{N}$ indirect detection and decoupling
HCP	triple resonance probe with proton ( $^1\text{H}$ ) on the observe coil and a double-tuned second coil for $^{13}\text{C}$ and $^{31}\text{P}$ indirect detection and decoupling
HF	Hartree-Fock (theory)
HFMRF	High-Field Magnetic Resonance Facility
HMEC	human mammary epithelial cells
HMGA1	high-mobility group protein
HOMO	highest occupied molecular orbital
HP	Hewlett-Packard
HPLC	high-performance liquid chromatography
HPMSF	High-Performance Mass Spectrometry Facility
HR	homologous recombination
HR-TEM	high-resolution transmission electron microscopy
HREELS	high-resolution electron energy loss spectroscopy
HRXRD	high-resolution x-ray diffraction
HX	double resonance, solid-state probe with proton ( $^1\text{H}$ ) decoupling and tunable observe coil
HXY MAS	triple resonance, solid-state, magic angle spinning probe; proton decoupling and tunable frequency ranges for mid-level (X) and low-gamma (Y) nuclei
I&NS	Interfacial & Nanoscale Science
ICP	inductively coupled plasma
IDA	Information Dependent Acquisition
IDL	Instrument Development Laboratory
IMAC	immobilized metal affinity chromatography
IR	infrared
IST	isotope-coded solid-phase tag
ITMS	ion trap mass spectrometry
LC	liquid chromatography
LDA	local-density-approximation
LDAP	Lightweight Directory Access Protocol
LEED	low energy electron diffraction

LET	linear-energy-transfer
LPS	lipopolysaccharide
LTA	Linde Type A
LUMO	lowest unoccupied molecular orbital
MAS	magic-angle-spinning
MBE	molecular beam epitaxy
MD	molecular dynamics
MDS	metadata server
MM	molecular-mechanical
MOCVD	metal organic chemical vapor deposition (system)
MOSFET	metal oxide semiconductor field-effect transistor
MOKE	magneto-optical Kerr effect
MP	membrane protein
MPP2	High-Performance Computing System-2
Mr	molecular mass
MRI	magnetic resonance imaging
MS	mass spectrometry
MSCF	Molecular Science Computing Facility
MS/MS	tandem mass spectrometry
MTSL	methanethiosulfonate
NAA	neutron activation analysis
NAPL	nonaqueous phase liquid
NBED	nanometer beam electron diffraction
NESG	Northeast Structural Genomics Consortium
NEXAFS	near-edge x-ray absorption fine structure
NIH	National Institutes of Health
NIR	near-infrared
NMDA	N-methyl-D-aspartate
NMR	nuclear magnetic resonance
NOE	nuclear Overhauser enhancement
NOESY	nuclear Overhauser enhancement spectroscopy
NRA	nuclear reaction analysis
NTP	nucleoside triphosphate
NWChem	Northwest Computational Chemistry
OD	outside diameter
OPA MBE	oxygen-plasma-assisted molecular beam epitaxy (MBE)
ORF	open reading frame
OS	operating system
Osp	outer surface proteins
OST	object storage target
PA	photo acoustic
PAGE	polyacrylamide gel electrophoresis
PAN	peroxyacetyl nitrate
ParSoft	Parallel Software Development Tools

PASS	phase-altered spinning sidebands
PCR	polymerase chain reaction
PDA	personal digital assistant
PDB	Protein Data Bank
PESA	proton elastic scattering analysis
PHI	Physical Electronics Instruments
PhIAT	phosphoprotein isotope-coded affinity tag
PhIST	phosphoprotein isotope-coded solid-phase tag
PiCEIS	Parallel Computational Environment for Imaging Science
PIGE	particle induced gamma emission
PIXE	proton induced x-ray emission
PME	phosphomonoesters
PMT	putative mass tag
PNNL	Pacific Northwest National Laboratory
ppb	parts per billion
ppm	parts per million
PRISM	Proteomics Research Information and Management System
PTFE	polytetrafluoroethylene
PTM	post-translational modifications
PTR	proton transfer reaction
QCO	quartz crystal oscillators
QM	quantum-mechanical
QMS	quadrupole mass spectrometer
QNP	quad-nucleus probe that can be switched among $^1\text{H}$ , $^{31}\text{P}$ , $^{13}\text{C}$ , and $^{15}\text{N}$
RAID	Redundant Array of Independent Disks
RBS/C	Rutherford backscattering spectrometry/channeling
RDC	residual dipolar coupling
REDOR	rotational echo double resonance
RF	radio frequency
RHEED	reflection high-energy electron diffraction
RNA	ribonucleic acid
R-NMRI	relaxation nuclear magnetic resonance imaging
RNP	ribonucleoprotein
SAC	Science Advisory Committee
SAED	selected area electron diffraction
SAM	self-assembled monolayer
SAMMS	self-assembled monolayer on a mesoporous support
SAN	Storage Area Network
SAS	surface analysis system
SCM	surface complexation model
SCR	selective catalytic reduction
SCX	strong cation exchange
SEM	scanning electron microscopy
SGE	Scalable Graphics Engine
SGI	Silicon Graphics Incorporated

SIC	self-interaction correction
SiC	silicon carbide
SID	surface-induced dissociation
SIMS	secondary ion mass spectrometry
SMP	symmetrical multiprocessing
Spm	superparamagnetic
ss	solid-state
SS	source-to-sample
STIM	scanning transmission ion microscopy
STM	scanning tunneling microscopy
STOMP	Subsurface Transport Over Multiple Phases
SW	short wave; short wavelength
T	telsa
TAC	Time to Amplitude Converter
TCSPC	time-correlated single-photon counting
TEM	transmission electron microscopy
TEY	total electron yield
TIC	total ion chromatogram
TIGR	The Institute for Genetic Research
TMD	transmembrane domain
TNT	trinitrotoluene
TOF	time-of-flight
TPB	tributyl phosphate
TPD	temperature-programmed desorption
TPSF	temporal point spread function
TST	transition state theory
UAC	User Advisory Committee
UHV	ultra-high vacuum
UPS	ultraviolet photoemission
USO	User Services & Outreach
UV	ultraviolet
UXO	unexploded ordinance
VSM	vibrating sample magnetometer
XAFS	x-ray absorption fine structure
XANES	x-ray absorption near-edge structure
XAS	x-ray absorption spectroscopy
XMCD	x-ray magnetic circular dichroism
XPD	x-ray photoelectron diffraction
XPS	x-ray photoelectron spectroscopy
XRD	x-ray diffraction
XRPD	x-ray powder diffraction
XRR	x-ray reflectivity