

12/20/2004 22:22				
CHE Cyber Workshop 10/3-5/04				
Sun.:				
Holiday Inn				
7:00 PM	Refreshments			
7:30 PM	Celeste Rohlifing	Welcome & Logistics		
7:40 PM	Art Ellis	Welcome		
7:50 PM	Teresa Head-Gordon & Mark Gordon	Welcome		
8:00 PM	Kim Baldrige	"Towards a Common Cyber-Enabled Computational Chemistry: Data Representation, Scientific Workflow, & Grid Computing"		
8:30 PM	Jesus Izaguirre	"BioCoRE: Cyber-Enabled Biochemistry"		
9:00 PM	Seth Pinsky	"Chemical Informatics for Industry and Academia: The Role of Commercial Software and Databases"		
9:30 PM	Thanh Truong	"Computational Science & Engineering Online: Progress and Perspectives"		
Mon.:				
Rm. 375				
8:00 AM	Refreshments @ Rm. 375 (available all day)			
8:30 AM	Sang Kim	Welcome		
Breakout Rms.		Comp. & Exptl.		Grand Challenge
	Core Chem.	Chem. at the Interface	Chem. Interactions	Chem.
9:00 AM	Rm. 375	Rm. 1060	Rm. 370	Rm. 320
(chair)	Todd Martinez	Julia Rice	Joe Francisco	Martyn Guest
(co-chair)	Theresa Windus	Jim Kubicki	Ken Jordan	Chris Cramer
	Thanh Truong	Terry Stouch	Seth Pinsky	Kim Baldrige
	Tom Holme	Howard Bilofsky	Anne Chaka	Alistair Rendell
	Ricky Kendall	Jesus Izaguirre	Alanah Fitch	Thom Dunning
	Neil Ostlund	Jeffry Madura	Will Polik	Jim Myers
	Jean Standard	David Whisnant	Jeff Nichols	Glenn Martyna
	Mike Colvin	Nancy Amato	Mike Frenkel	Susan Sinnott
	John Harkless	David Kofke	Marti Head	Sharon Glotzer
	Steven Rick	Kirby Vandivort	Jay Ponder	Michael Mahoney
			Chris Roland	Celeste Sagu

Lunch 12 N					
Rm. 375					
2:00 PM	Shenda Baker	"MPS Cyber Workshop Report"			
Breakout Rms.			Databases &	Education &	
	Software & Algorithms	Hardware Infrastructure	Cheminformatics	Training	Remote Chemistry
2:30 PM	Rm. 375	Rm. 1060	Rm. 370	Rm. 320	Rm. 920
<i>(chair)</i>	<i>Sharon Glotzer</i>	<i>Ricky Kendall</i>	<i>Anne Chaka</i>	<i>Tom Holme</i>	<i>Thom Dunning</i>
<i>(co-chair)</i>	<i>Susan Sinnott</i>	<i>Jeff Nichols</i>	<i>Jeffry Madura</i>	<i>Will Polik</i>	<i>Alanah Fitch</i>
	Alistair Rendell	Todd Martinez	Howard Bilofsky	Neil Ostlund	Kim Baldrige
	Jesus Izaguirre	Chris Cramer	Seth Pinsky	David Whisnant	Glenn Martyna
	Jay Ponder	Martyn Guest	Joe Francisco	David Kofke	Shenda Baker (PM only)
	Theresa Windus	Julia Rice	Marti Head	John Harkless	Jim Myers
	Michael Mahoney	Mike Colvin	Mike Frenkel	Jean Standard	Ken Jordan
	Kirby Vandivort	Terry Stouch	Jim Kubicki	Thanh Truong	Steven Rick
	Nancy Amato	Chris Roland	Celeste Sagui		
Tues. AM:					
Rm. 375					
8:00 AM	Refreshments @ Rm. 375				
8:30 AM	Reports from 4 Monday Morning Breakout Sessions				
10:00 AM	Break				
10:20 AM	Reports from 5 Monday Afternoon Breakout Sessions				
12:00 PM	Adjourn				