Energetic Materials/Insensitive Munitions Joint MURI Review
11-13 July 2006
The Officers Club
Aberdeen Proving Ground, MD

<u>Please note:</u> We are incorporating breakout sessions within the review format, to promote an informal exchange of ideas between MURI investigators and Army researchers, and a workmanlike approach to problem solving. The breakout schedule is extremely flexible, so you may be asked to participate, or you may ask to participate in a session.

Tuesday - 11 July 2006

8:00 Bob Shaw, Army Research Office
Introduction
8:50 David Ceperley University of Illinois Urbana-Champagne
Quantum Simulations of Materials Under Extreme Conditions
Breakout Session – Don Thompson, Univ. of Missouri (session leader – Rice)
9:40 Rod Bartlett, University of Florida
Ab-Initio Predictions of PES for Chemical Reactions
Breakout Session – Ceperly, UIUC (session leader- Mattson/Romero)
10:30 Break
10:45 Herman Ammon, University of Maryland
Structure and Density Predictions for Energetic Materials
Breakout Session – Bartlett, UF (session leader – Byrd/Taylor)

11:30 Lunch – APG Officers Club

1:00 Don Brenner, North Carolina State Univ.
Condensed Phase Energetic Materials: A Bridge Between Ab Initio Calculations And Experimental Shock Dynamics
Breakout Session – Chamberlin, UIUC (for Truhlar/Cramer (session leader – Hurley)
1:50 Don Thompson, University of Missouri-Columbia
Simulations of Physical/Chemical Processes in Gas/Liquid/Solid Phases
Breakout Session – Brenner,NCSU (session leader – Rice)
2:40 John Adams, Univ. of Missouri - Columbia
Flame-Surface Heat Exchange
Breakout Session – Brenner,NCSU (session leader – Rice)
3:30 Break
3:45 Adam Chamberlin, Univ. of Minnesota
Progress Towards an Accurate and General Model for the Solubility of High-Energy Compounds in Supercritical Solvents
Breakout Session – Adams, UM-C (session leader – Rice)
4:30 Bob Shaw, Army Research Office
Discussion/Closing Remarks

Wednesday - 12 July 2006

8:15 Kevin McNesby, Army Research Office/Army Research Laboratory
Introduction
8:30 Bill Goddard, CalTech
Overview of Accomplishments and Goals
8:45 Adri van Duin, Caltech
Progress In Developing Reaxff For Describing Reactive Processes In EM Materials And Also In Catalysis, Ceramics, And Metallic Systems
9:15 Sergey Zybin, Caltech
Applications Of Reaxff To Shock And Thermal Impact Studies Of EM. Dependence On Orientation And Phase And Formation Of Clusters
9:45 Break
10:00 Aiichiro Nakano, Univ. of Southern California
Multi-Million Atom Simulations Of Energetic Materials
Breakout Session – Malcolm Nicol , UNLV (session leader – Ciezak)
10:30 Eric Surber, Univ. of Illinois Urbana-Champagne
Sum Frequency Generation Characterization Of The Surface Structure Of HMX
Breakout Session – Aiichiro, USC (session leader – Mattson)
11:00 Tahir Cagin, Texas A&M Univ.
Nonlinear Elastic Constants From First Principles QM
Breakout Session – Surber, UIUC (session leader – Ciezak/McNesby)
11:30 Lunch APG Officers Club

1:00 Malcolm Nicol, University of Nevada Las Vegas
Overview
1:30 Oliver Tschauner Univ. of Nevada, Las Vegas
Shear Induced Transition in PETN – Structure of New Phase
Breakout Session – Zybin, van Duin, Caltech (session leader – Rice/Andzelm)
1:45 Michael Pravica, Univ. of Nevada, Las Vegas
Radiation Damage Studies of TATB and PETN
Breakout Session – Zybin, van Duin, Caltech (session leader – Rice/Andzelm)
2:00 Przemek Dera Univ. of Nevada, Las Vegas
New Approaches to Single-Crystal Diffraction
Breakout Session – Zybin, van Duin, Caltech (session leader – Rice/Andzelm)
2:15 B Yulga, Univ. of Nevada, Las Vegas
Spectra and Structure of HFNX
Breakout Session – Zybin, van Duin, Caltech (session leader – Rice/Andzelm)
2:30 Break
2:45 Maija Kukla, NSF
Overview And Progress Report On Simulation And Theory Projects
Breakout Session – Zybin, van Duin, Caltech (session leader – Rice/Andzelm)
3:15 Ivan Oleynik, Univ. South Florida
First-Principles Modeling of Energetic Materials
Breakout Session – Zybin, van Duin, Caltech (session leader – Rice/Andzelm)

3:30 Sergey Rashkeev, Vanderbilt Univ.
Shear-Induced Modeling in FOX-7 and TATB
Breakout Session – Zybin, van Duin, Caltech (session leader – Rice/Andzelm)

3:45 Alexander Roytburd, Univ. of Maryland
Polymorphic Transitions under Extreme Stress
Breakout Session – Zybin, van Duin, Caltech (session leader – Rice/Andzelm)

4:00 Discussion
Breakout Session – Nicol Theoretical Team (session leader – Rice)

Thursday - 13 July 2006

8:00 Kevin McNesby, Army Research Office/Army Research Laboratory
Introduction
8:05 Don Thompson, University of Missouri-Columbia
Overview - UM-C Team Multiscale Modeling
8:30 Steve Stuart, Clemson Univ.
Reactive Potential Development
Breakout Session – (session leader – Rice/Andzelm)
9:15 Tommy Sewell, LANL
Atomistic-Based Mesoscopic Constitutive Models for High Explosive Constituent Materials
Breakout Session – Stuart, Clemson (session leader – Rice/Andzelm)
10:00 **Break**
10:15 Don Brenner, North Carolina State Univ.
Multiscale Modeling
Breakout Session – Sewell, LANL (session leader – Rice/Andzelm)
11:00 Don Thompson, University of Missouri-Columbia
MD Simulation Methods
Breakout Session – Brenner, NCSU (session leader – Rice/Andzelm)
11:30 **Discussion**
12:00 Kevin McNesby/David Mann, ARO
Concluding Remarks