Computational Materials Theory Program Overview

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Objectives of Program Overview

What brings us together today?

- Impossible to visit all
- Participants represent all larger and initiative-supported research projects
- Diverse group representative of Materials Theory (plus a bit of CMP experimental QIS research)
- Opportunity to present your research to NSF and peers
- Encourage cross-talk
- Student and postdoc participation
- Underline future opportunities for MT community through ITR and NSE
Materials Theory

- Provides support for theory, modeling and simulation which spans DMR (condensed matter theory, theoretical materials science and solid state chemistry)
- Provides support for theoretical topics funded in other DMR programs, i.e., if it is supported in DMR, MT will support the theory
- Does not explicitly fund experimental research, although experimental connections are important
- Advances methodologies and techniques. e.g., algorithms, formal methodologies, mathematical methods
- Nurtures an integrated ‘Materials Theory’ community
Advanced Computation in DMR

- Condensed Matter Theory Program 1972
- Materials Theory Program 1990
- Cohen and Louie; Ceperley and Martin
- Atomistic approach to materials modeling
- HPCC/CARM 1992 & 1995
- KDI 1998 & 1999
- ITR 2000-2004 (Small, Medium and Large)
- NSE 2001-2005 (NER, NIRT, NSEC)
- FRG
- Many smaller, individual investigator grants
Materials Theory Infrastructure

- Institute for Theoretical Physics, UCSB
- Aspen Center for Physics
- Materials Computation Center, UIUC
- Boulder Summer School on Condensed Matter and Materials Physics, Colorado
- Workshop on Opportunities in Materials Theory, NSF (Oct 14-16, 2002)

Additional Centers with a Computational Thrust ??
Budgetary Trends and Future Funding Opportunities

Discretionary budgets are under extreme pressure:

*Decreasing, Little Flexibility, Minimize Damage*

‘Window of opportunity’ for the MT community

- **NSE Initiative** - *three more years*
  - Broad support for science on the ‘nanoscale’

- **ITR Initiative** - *two more years*
  - **FY01**: ‘APPLICATIONS IN SCIENCE AND ENGINEERING’ - simulation, modeling, etc. & ‘SYSTEMS DESIGN AND IMPLEMENTATION’ - revolutionary computing
  - **FY02**: ‘SCIENTIFIC FRONTIERS AND INFORMATION TECHNOLOGY’ - simulation, etc. & “revolutionary computing”

Will the next initiatives be so ‘friendly’ to MT?
MT is interested in using this opportunity to enhance computational research at *all levels*
Opportunities for MT Community

- Enhance support of individual investigators in computational areas
  - ITR Small ($500,000 Max, typ. 3 years)

- Enhance support of collaborative research efforts (“FRG’s”)
  - NSE: NIRT (up to $2 Million for 4 years -- 3 or more PI’s)
  - ITR: ITR Medium ($5 Million Max, 5 years)

*Room for computation + analytical theory, expt., ...*
Opportunities for MT Community

- **Enhance MT infrastructure**

  Center for Computational “X” with X = soft condensed matter, many-body physics, electronic structure, materials science, quantum computing, biomolecular materials, etc., AND interactions among them, e.g., many-body theory and electronic structure

  - **ITR Medium** ($5 Million / 5 yrs) -- greater flexibility
  - **ITR Large** ($15 Million/ 5yrs) -- Pursue with caution!
Strong ITR Proposals

- General: Strongest proposals usually have
  - an interdisciplinary character
  - strong education components (undergraduates, graduates, postdocs and diversity)

- Center (medium): Speaks to the needs of the broader community
  - How does it fit in the MT community?
  - Respects the master relation!
    Whole > Sum over parts
  - Collective vs. Competitive

Acknowledge the efforts of your peers!