

## Minutes of the VC meeting on 'Material Science / Nano technology'

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Moderator – Dr. B.P.Das IIAP and Dr.Sundararajan (C-DAC)

Date and Time – 04 Mar 2008 - 2 PM to 2:45 PM

1. List of participants:

Prof. B.P. Das, Dr. Sunder Rajan (C-DAC-Pune), Dr. Devendra Sharma (IPR),  
Dr. Tapan Mishra (IIAP), Ms. Janaki (C-DAC-Bangalore)

2. It was generally felt that atomic, molecular, materials and nanoscience could be the broad areas of virtual community

3. List of interested institutions and representatives:

IIAP -- B.P. Das, Tapan Mishra, H.S. Natataj, Meetu Sethi

C-DAC -- Dr. V. Sundararajan

NCL -- Dr. S. Pal

PRL -- Dr. Angom Dilip

IPR -- Dr. Devendra Sharma / Dr. Subrat Mukherjee

IISc Dr. Shenoy, Prabal Maity

Univ Of Pune - Prof. Kanhere

Univ of Hyd - Prof. Shastry and KPN. Murthy

SINP - D. Bhattacharya (to be contact)

IITK - R. Prasad

BARC - Swapan Ghosh, C. Majumder

IACS (not partner) - G.P. Das, and D. Mukherjee

JNCASR ... - Waghmare, S. Bala, Shobana Narasimhan, Swapan Patti

SNBose - A Mookherjee, Tanushree Saha Dasgupta

4. Kinds of activities / requirements:

1. Standard codes list: CPMD, PARSEC, CCSD, Relativistic CCSD, GAMESS, GAUSSIAN

2. CPU and memory intensive compute applications

3. Visualization tools:

5. Possible action items:

1. A mailing list of members, Repository of codes, tools within the group

2. Sharing of results and publications, Video conferencing and telecasting of events

3. Identification of a grand challenge problem (requiring computation) for the whole group or few of the partners:

a) Relativistic CCSDT for heavy atoms  $z > 55$

b) Quantum dot simulations of 200 to 1000 atoms

c) Applications of DMRG to cold atoms

6. Resource requirement (from Garuda) to be drawn-up based on the above, e.g.

1. Requirements for video conferencing

2. Do we have the resources for chat or some other communication tool over Garuda

3. Requirements for repositories of tools, publications etc

4. Minimum of 64 CPUs and preferably more on a single cluster of a grid node.