

# Story of Crystallographic Research in India: A Tribute

*In celebration of International year of  
crystallography*

T Ramasami

Ministry of Science and Technology, Gol, New  
Delhi

# Research in Crystallography in Modern India: Some key milestones

---

- K Banerjee determined the crystal structure of naphthalene in 1930s
- Two students of Sir CV Raman initiated diffraction of X Ray by crystals 1940s
  - Ramaseshan built the school in crystallogrchy
  - Ramachandran became the founder of structural biology in India
- Professor Hodgkin remarked once in 1980s that India herself came to be recognized by her for the contributions to X-Ray Crystallography

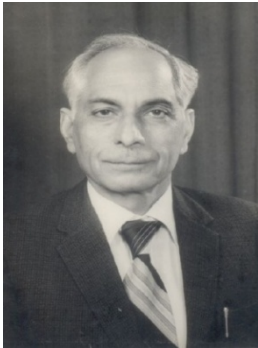
An attempt will be made to capture a story and pay a tribute to the story makers

# Milestones



K. Banerjee

- \* Published crystal structures of naphthalene and anthracene (Indian Association for the Cultivation of Science, 1929).
- \* Proposed direct method of the crystal structure determination with William Henry Bragg (1933).



A. R. Verma

- \* Worked on unimolecular growth spirals on the surfaces of crystals (University of London, 1946-1952) .
- \* Authored a book with P. Krishna titled “Polymorphism and Polytypism in Crystals (1966)”.



G. N. Ramachandran

- \* Proposed a triple-helical model for the structure of collagen (Madras University, 1954).
- \* Ramachandran plot for understanding conformation of peptide structures (Madras University, 1963).



S. Ramaseshan

- Solved crystal structure of  $\text{KMnO}_4$  suggesting the idea of multiple wavelength phase determination (Indian Institute of Science, 1953).

- \* Contributions to the development of anomalous scattering methods (Oxford University, 1965).



R. Chidambaram

- \* Published “bent hydrogen bond model in the structure of ice-I” (Indian Institute of Science, 1962).

- \* His paper on “The crystal structure of potassium oxalate monohydrate: lone-pair coordination of the hydrogen bonded water molecule in crystals” is cited over 200 times (BARC, 1962).

- \* His research was on solution of the phase problem in crystals with centre of symmetry, using the phenomenon of anomalous dispersion effects (Indian Institute of Science, 1955).

- \* Co-authored a book “Computing in *Crystallography*” with R. Diamond and S. Ramaseshan (Indian Institute of Science, 1980).



K. Venkatesan



M. Vijayan

- \* Worked on the crystal structure and carbohydrate specificity of lectins and protein hydration (Indian Institute of Science, 1994-2004).
- \* Contributed on the structure and interactions of mycobacterial proteins and supramolecular association.



G. R. Desiraju

- \* Pioneer of Crystal Engineering (University of Hyderabad, 1989).
- \* Proposed the concept of the supramolecular synthon (University of Hyderabad, 1995).
- \* Co-authored a book entitled “The Weak Hydrogen Bond In Structural Chemistry and Biology” with T. Steiner (2001).

**There have been many more and important contributions emanating from India. Some of them have become global landmarks stimulating further interest in the area. I pay tribute to those who made India an important center for crystallography**

# An Inspiration from the master: Work on Collagen

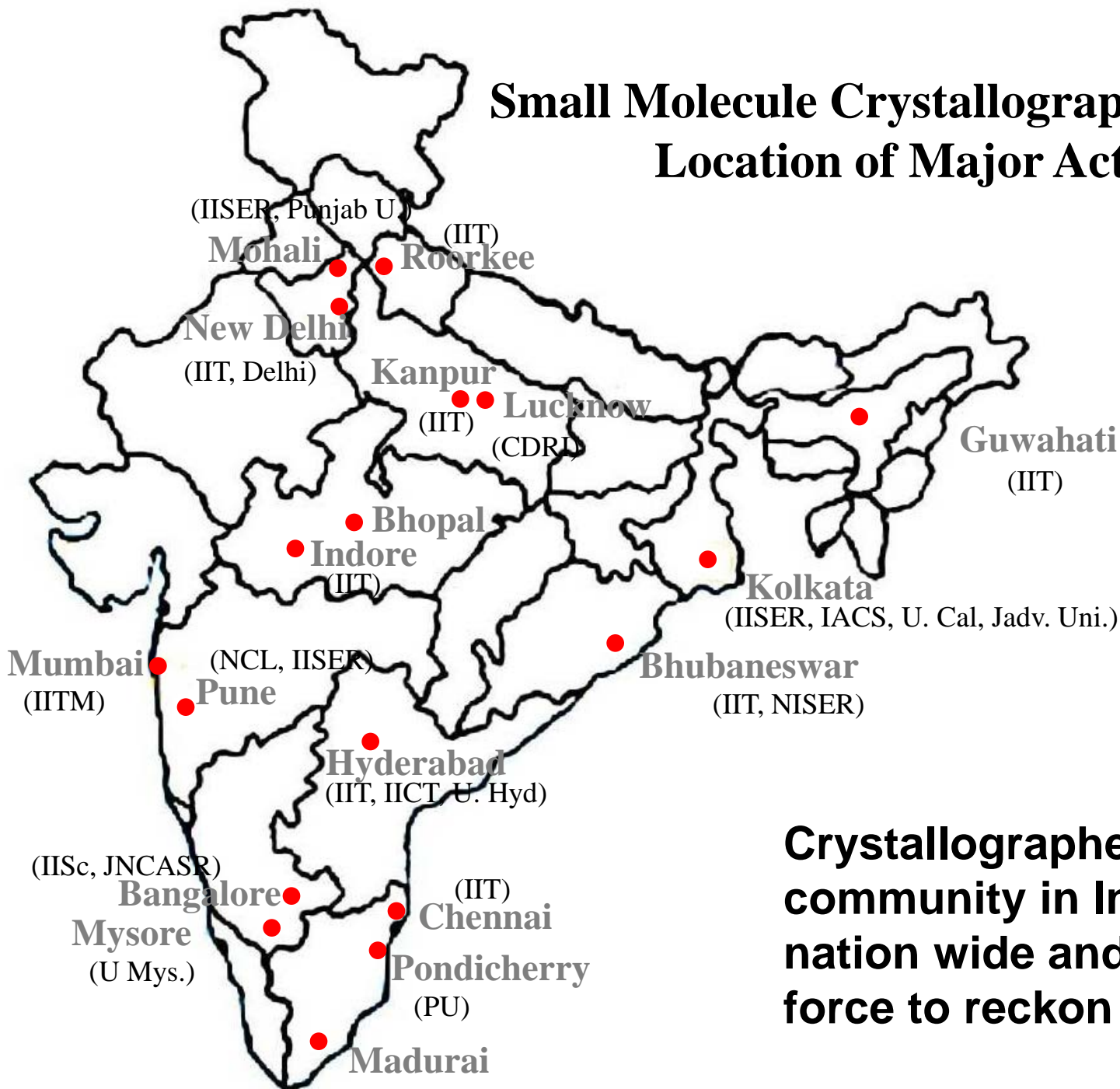
---

- Prof GN Ramachandran and his group chose to study the structure of collagen. He had a neighbor (CLRI) for whom collagen formed the main material for work
- Madras Triple helical structure of collagen with 2 hydrogen bonds pre triplet was reported on 7 August 1954.
- Critics posed some conformational arguments against Madras model
- Ramachandran plot was developed. It is a case of theory preceding experiments and proving the test of time
- He opened the concept of image reconstruction.



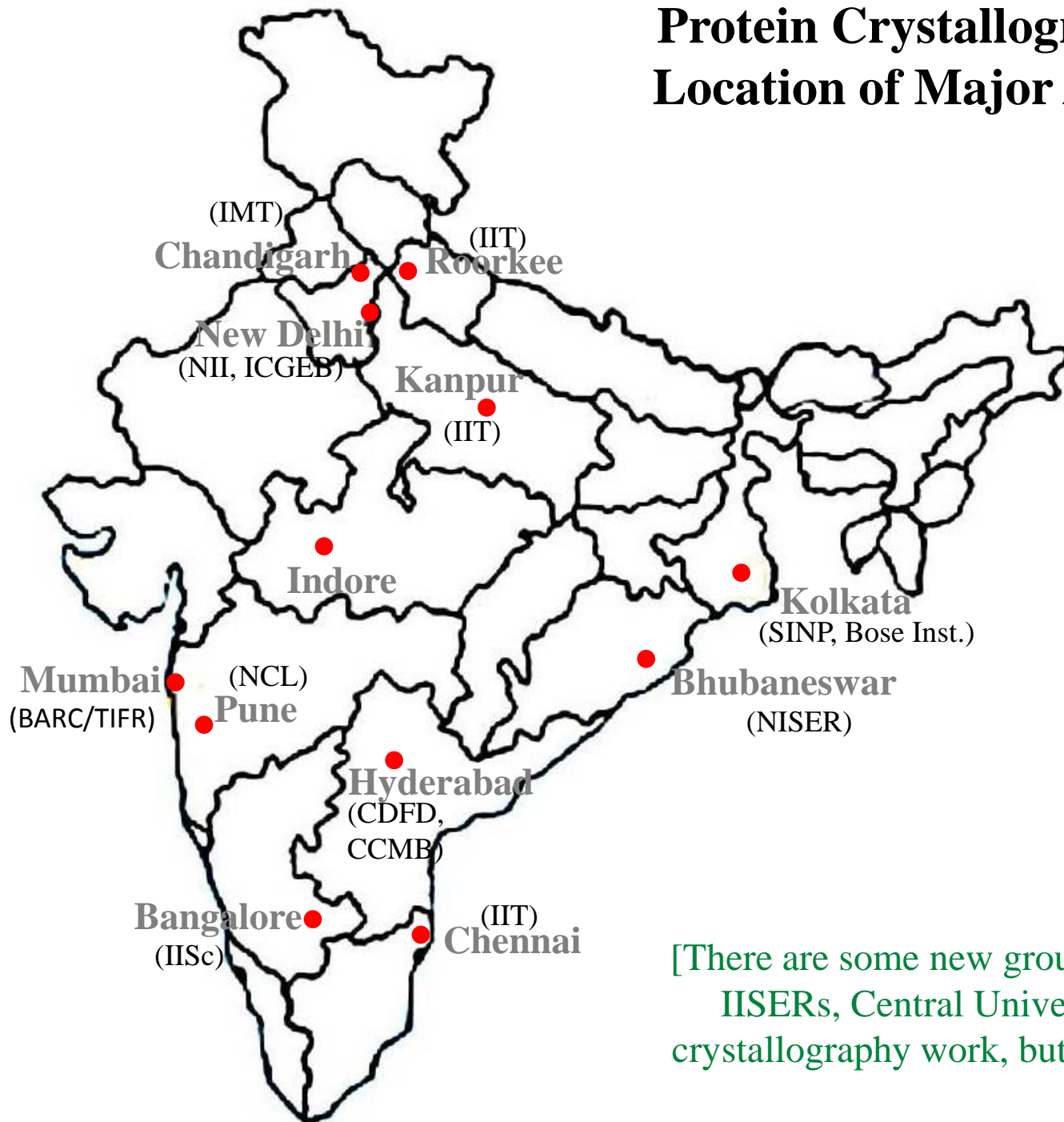
GNR has been a giant among the giants of structural biology. Collagen was blessed by his work. This talk is dedicated to the spirit of perfection in the creative genius of GNR.

# Small Molecule Crystallography in India: Location of Major Activity



**Crystallographer  
community in India spread  
nation wide and emerged a  
force to reckon with**

# Protein Crystallography: Location of Major Activity



[There are some new groups in new institutes (IITs, IISERs, Central Universities), started protein crystallography work, but all are not included here]



# Single Crystal X-Ray diffractometers in India

1977

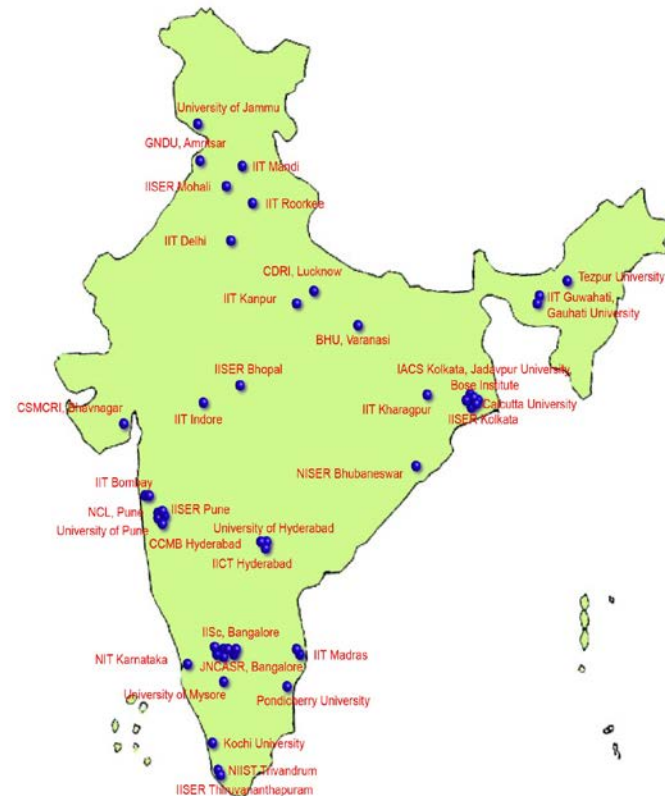
1977,1979,1987

2014

IISc, Bangalore



Funding has impacted the Growth of the community of crystallographers



# Chronology of Chemical Crystallography: Some Milestones

---

**1977**  
Organic/inorganic  
Structures  
(IISc)

**1983**- C–H....O  
Hydrogen bonding  
UoH

**1989**- Crystal  
engineering  
(UoH).

**1995**-  
Supramolecular  
Synthons (UoH)

**1997**- Coordination  
polymers and metal-  
organic frameworks  
(IACS)

**2006**- Pharma  
Cocrystals & salts &  
property modification  
(UoH)

**IISc: Indian Institute of Science, UoH University of Hyderabad;**  
**IACS: Indian Association of Cultivation of Science**

# Crystallographic Research in Modern India: From the perspective of MoST

---

- Competitive Research grant models were developed and positioned in India in 1974 and in more recent times a new autonomous body (SERB) created through an Act of Parliament has become fully functional
  - A Review of outcome of R&D funding reveals that
    - Structural biology is one of the areas benefiting from planned R&D support
    - Chemical crystallography with insight from chemists started in the late 1970s
    - With increasing support for single crystal X-ray diffractometers after 2000s, crystal engineering has prospered in India
- India has invested recently on gaining access to synchrotrons in the world
  - Indian beam line in Japan, access to Petra, Elettra, Grenoble etc.
  - A proposal mooted for establishing a second Facility in India

# New Vistas in crystallography

---

- Ordering in molecular systems seems to influence the functional behavior of supra molecular assemblies
- Insight into crystallography seems to aid in designing and developing new materials with designer properties and functional applications
- New Vistas in crystallography make the crystallographers the molecular architects of modern era. A self Assembly of crystallographers is evidenced

# Increased International S&T Cooperation

A case for new models

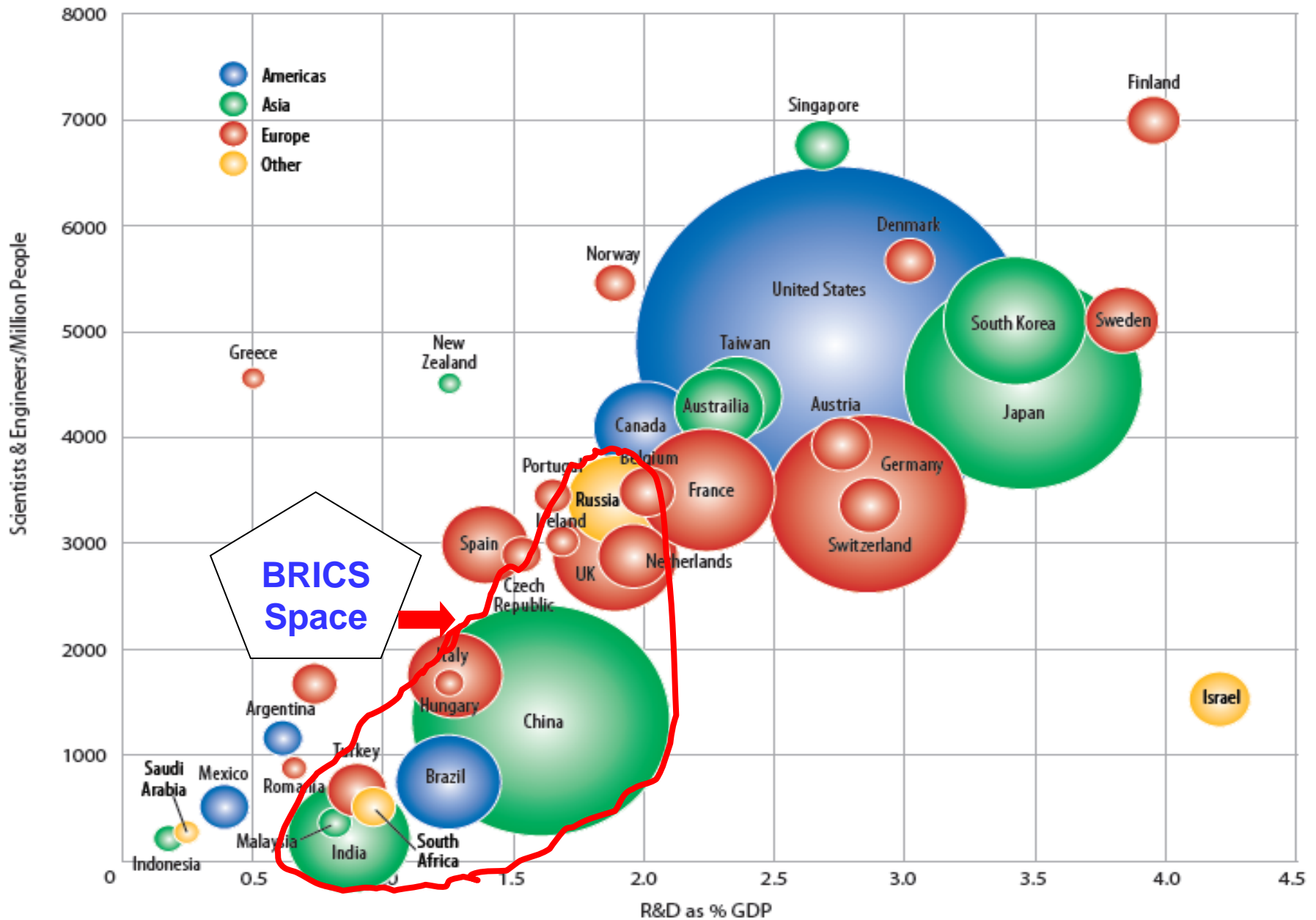
# Collaborative Excellence in basic research

---

- Traditionally basic research in the world had been driven by human passion to know more and earlier than others
  - Raman was able to perform his Nobel prize discovery through home built instrument. Concept driven research was built on the grammar of competitive excellence
- Nation states invested heavily on a competitive mode
- Research in modern times is enabled by large R&D infrastructure which is becoming beyond the investment capacities of Nations
  - Is collaborative excellence with co investment into creation of large infrastructure for R&D a new model?

# World of R&D 2011

Size of circle reflects the relative amount of annual R&D spending by the country noted.



Source: Battelle, R&D Magazine, International Monetary Fund, World Bank, CIA World Factbook, OECD

# Collaboration in crystallography: Way forward for BRICS

---

- Crystallography, today has become a collaborating platform for mathematicians, physicists, chemists, biologists, engineers and technologists and discoverers of drugs as well as pharmaceutical industry. Crystal engineering is an active area for cross fertilization of ideas.
- Creation of large R&D infrastructure for engineering structures of designer properties measurements of parameters as well as deployment of modern crystallography is an area for future collaboration among BRICS countries
- A special task force of say 10 experts for exploring collaboration among BRICS Nations in the area of crystallography may seem a good way forward



# Summary

---

1. India enjoys a tradition of research in crystallography
2. Some important leads emanating from India could be chronicled and tributes paid
3. Public investments in India in the field seem to have made some impact in the promotion of research in the area. Crystallographers seem to prosper.
4. A case is made for collaborative excellence in global R&D on crystallography
5. BRICS framework offers a unique opportunity for collaboration. It seems a way forward is to collaborate in this area and tap unique value in pharmaceutical industry and developing materials with designer properties

# Thank you

Acknowledgement: Professor Desiraju gave me significant amounts of inputs and even slides. Thank him for his thoughts and help.