WITS UNIVERSITY

100 1922 2022

# Richard Martin and the foundation of ASESMA

Nithaya Chetty

*Dean of Science*

*Professor of Physics*

*Vice President IUPAP*

Richard Martin

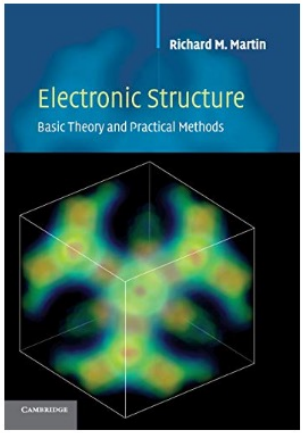
A global inspiration for science and humanity

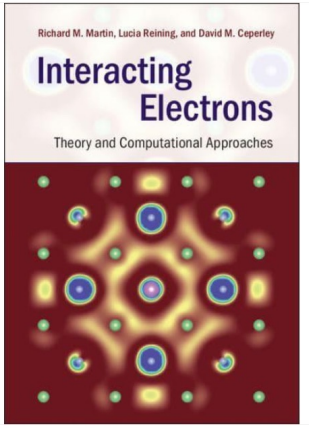
# Richard Martin has pioneered the field of Electronic Structure computations for over 50 years

- PhD U. Chicago 1969

- Appointments
  - Bell Labs 1969-1971
  - PARC 1971-1987
  - Stanford 1986-1989
  - U. Illinois 1987-2007

- Honours
  - Von Humboldt Foundation Senior Scientist Award.
  - Fellow, American Physical Society
  - Fellow, American Association for the Advancement of Science.
  - NSF Graduate Fellow 1964-9
  - Fellow of the SAIP



# The prevailing conditions 15 years ago

- The environment for ASESMA to be established was perfect
- There was/is a need for
  - Science development in Africa
  - Low investments in S&T by African governments
  - Large-scale networking, collaborations and connections within Africa
  - Low cost but high quality education and research endeavour
- ICTP has had a historic involvement in Africa
- IUPAP had a growing interest in Africa
- There is a great amount of goodwill shown by the international Science community toward scientific development in Africa
- Lots of untapped intellectual talent in Africa

# ASSEMA is the confluence of different efforts

International Union for Pure and Applied Physics (IUPAP)

The international Electronic Structure Community, including tutors

ICTP and Quantum Espresso developers

The African scientific community
- Thought leaders and students

International Organizations, funders and sponsors

Richard was central to many of these conversations
- If not central, then certainly inspirational

# Many people to thank

## - the early years

- Sandro Scandolo

- George Amolo
- Ali Hassanali
- Nicola Serani

- Paolo Giannozzi
- Stefano Girancoli
- Stefano Baroni
- Ralph Gebauer
- Matteo Gatti
- Nicola Manzzari

- Shobhana Narasimhan
- Mark Casida
- Renata Wentzcovich
- Sinead Griffin
- Allison Hyatt
- Garu Gebreyesus
- Ryo Maezono
- Nisha Mammen
- Andrea Marini
- Lucia Reining
- Omololu Akin-Ojo
- Steve Ndengue
- Iurii Timrov.

*… we have made something that has changed the way research is done in many fields of science and technology!*
*- Richard Martin 2022*

# Quick timeline

- Fulbright Fellowship to U. Illinois 1985-1990
- First met Richard Martin July 1987
- 1st PhD student of Richard's at U. Illinois
- Inaugural Workshop on Recent Developments in Electronic Structure (ES89)
- Richard and Beverly visited SA, DFT Summer School 1997
- Nithaya visited U. Illinois 2004
- Forerunner ASESMA 2008 at AIMS
- ASESMA 2010-2020, 2020-2030
- SAIP President 2007-2009
- IUPAP VP 2017-
- Richard Martin Fellow of the SAIP 2021


ILLINOIS

1997


ARCTIC OCEAN
Greenland
(Denmark)
Svalbard
(Norway)
ARCTIC OCEAN
United States
Canada
United States
Iceland
Norway
Sweden
Finland
Russia
U.K.
Den.
Neth.
Belg.
Ireland
Estonia
Latvia
Lithuania
Ger-
many
Poland
Belar.
Ukraine
Cz.
Mol.
Rom.
Bul.
Kazakhstan
Mongolia
Georg.
Az.
Armenia
Uzbek.
Turkm.
Kyrgyzstan
Tajikistan
ATLANTIC
OCEAN
Portugal
Spain
France
Italy
Turkey
Cyprus
Greece
Syr.
Lebanon
Iraq
Iran
Afghan.
Pakistan
China
N.Korea
S.Korea
Japan
Nepal
Bhutan
Kuwait
Qatar
Morocco
Tunisia
Algeria
Libya
Israel
Jordan
Saudi
Arabia
India
Laos
Vietnam
Taiwan
PACIFIC
OCEAN
Western
Sahara
Egypt
U.A.E.
Oman
Bur.
Bangl.
Thai.
Cambodia
Philippines
Mexico
Caribbean
Maurit.
Mali
Niger
Chad
Eritrea
Yemen
Djibouti
Senegal
Sudan
The Gambia
B.Faso
Guinea-Bissau
Guinea
Sierra Leone
Liberia
Cote d'Ivoire
Nigeria
C.A.R.
South
Sudan
Ethiopia
Sri
Lanka
Malaysia
Central
America
Guyana
Suriname
French
Guiana
(France)
Venez.
Colombia
Ecuador
Peru
Brazil
Cam.
Ghana
Benin
Togo
Equatorial Guinea
Gabon
Congo
Dem.
Rep. of
Congo
Ken.
Somalia
Uganda
Rwanda
Burundi
Tanz.
Papua
New Guinea
Indonesia
Solomon
Islands
Timor-Leste
Bolivia
Paraguay
Chile
Argentina
Uruguay
Angola
Zambia
Zim.
Bots.
Namibia
South
Africa
eSwatini
Lesotho
Malawi
Mozambique
Madagascar
INDIAN
OCEAN
Australia
New
Caledonia
Fiji
New Zealand

# The **True Size** of **Africa**

| COUNTRY | AREA x 1000 km² |
|---|---|
| China | 9.597 |
| USA | 9.629 |
| India | 3.287 |
| Mexico | 1.964 |
| Peru | 1.285 |
| France | 633 |
| Spain | 506 |
| Papua New Guinea | 462 |
| Sweden | 441 |
| Japan | 378 |
| Germany | 357 |
| Norway | 324 |
| Italy | 301 |
| New Zealand | 270 |
| United Kingdom | 243 |
| Nepal | 147 |
| Bangladesh | 144 |
| Greece | 132 |
| **TOTAL** | **30.102** |
| **AFRICA** | **30.221** |


- A vast and inhomogeneous continent with much diversity
- Anglophone, Francophone, Lusophone
- Different cultures, different indigenous languages, different histories, different geographies, different economies, different politics
- Not a one-size-fits-all

- Ravaged by slavery, colonialism, apartheid
- War, displacement
- Poverty, malnutrition, migration
- Inequality
- Political dictatorships
- Corruption
- Population growth
- Unemployment
- Under developed Infrastructure

African countries have a common destiny forged by closer cooperation within Africa, with support from the outside, with Science being central for development

**Africa** is very young

- 60% of the entire continent aged below 25yrs
- the youngest continent in relation to population

The greatest gift we can give our children is the opportunity to dream that anything is possible

# Need a nuanced and sustained approach

- Science as an instrument for development
- Not necessarily because the world owes it to Africa
- We need Africa to fully join the community of scientific nations for the well-being of all of humanity

- Many problems facing humanity are of a global nature
  - Affect people across the entire planet
  - Many impoverished countries face global issues disproportionally
    - Climate change, energy security, food security
    - Migration, brain-drain
  - Need for a stronger, collaborative international scientific community
  - Need to go a longer way to finding scientific-based solutions for the benefit of all of humanity

# Importance of material science in Africa

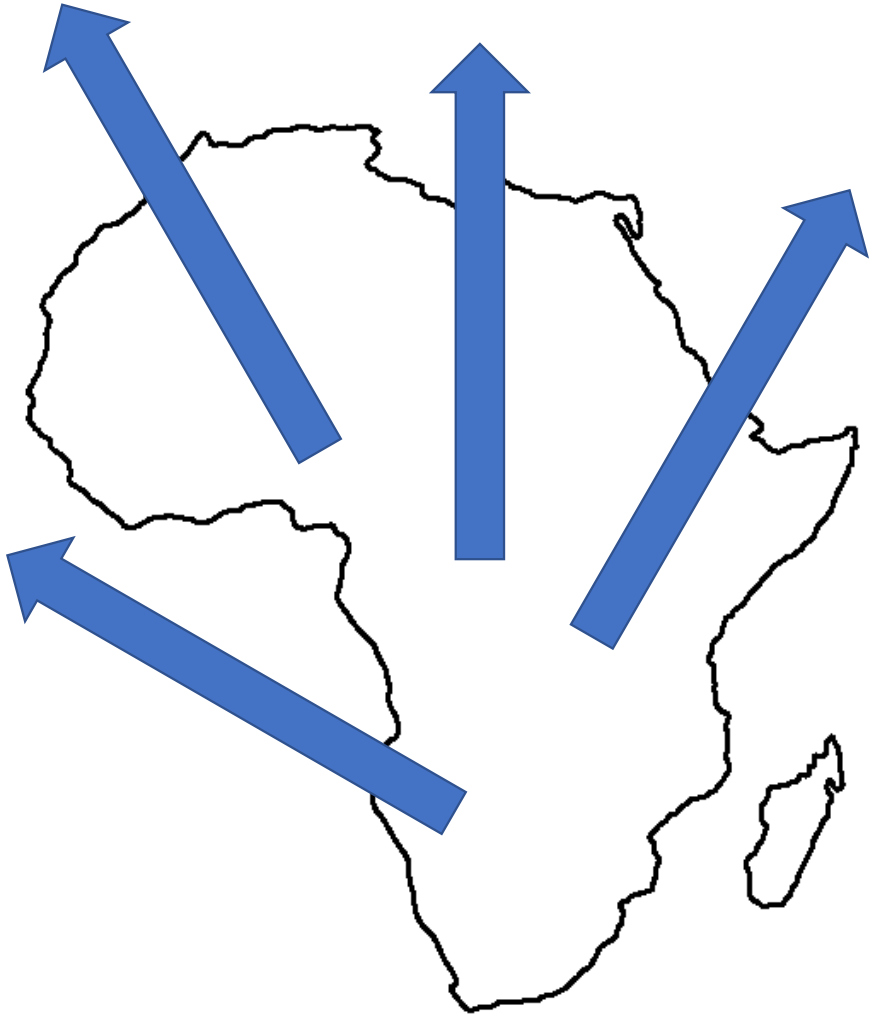
- Abundance of raw materials
  - Need to add more value
- Need a higher level material science research endeavour
  - Across all of Africa

- People
  - Not short of talent but we need to grow critical mass
  - Create more opportunities in Africa, stem brain drain
- Expensive equipment and infrastructure

# Electronic Structure Computations

- A great opportunity for Africa
  - Relatively cheap
  - Can interact remotely
- Very large community of people using Density Functional Theory for QM studies of Solids
  - Physics, Applied Maths, Chemistry, Material Science, Engineering, Biological Sciences
  - Industry
- Interests span
  - Education
  - Fundamental theoretical foundations
  - Computational algorithms and development
  - Practical applications

Scientific training and cooperation in and out of Africa



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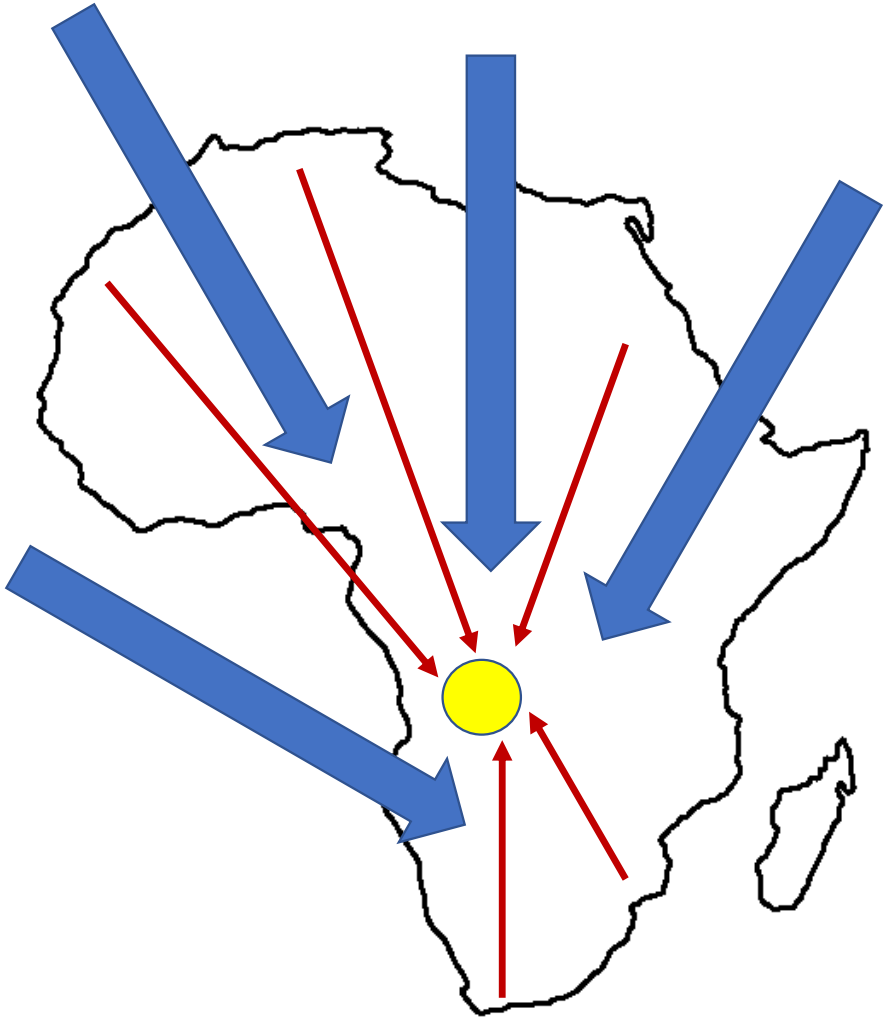


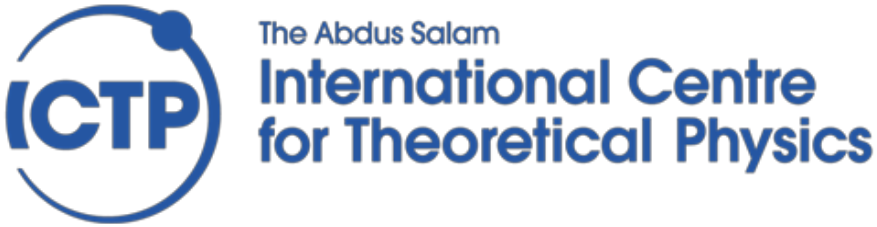
# The African School of Electronic Structure Methods and Applications (ASESMA)

- Began in 2008
- Richard Martin, Sandro Scandolo (ICT), Nithaya Chetty
- Jim Gubernatis, Kennedy Reed, Peter Borcherds (IUPAP)
- Biennial School Series in QM studies of real materials over 2 weeks
- Rotates through different African countries
- Lecturers, mentors from around the world including Africa

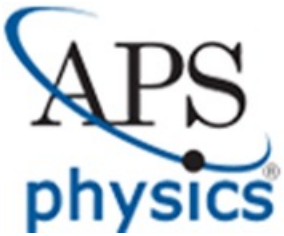
- Most work occurs in between Schools

Beijing Supercomputing Centre











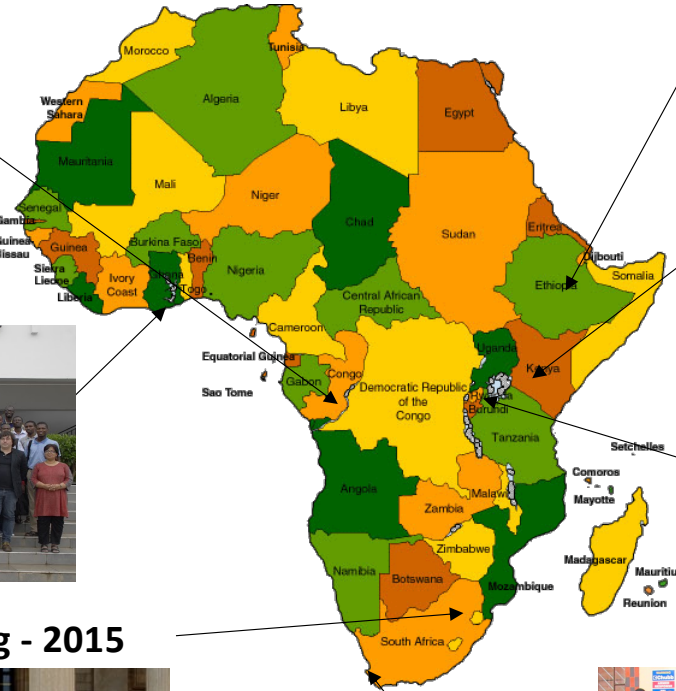



Materials Research Lab Santa Barbara

# ASESMA Schools

**Ethiopia - 2018**

**Mini-ASESMA**
**Rep. of Congo**




**Kenya - 2012**

**Ghana - 2016**

**Rwanda - 2021, 2023**

**Johannesburg - 2015**

**Capetown**
**– 2010**

USAfri

APS Innovation Fund



## About the U.S.-Africa Initiative in Electronic Structure

**The U.S.– Africa Initiative in Electronic Structure (USAfri)** aims to create a platform for exchange between African and U.S. physicists with opportunities to have a major impact on research and education in Africa. Electronic Structure is a natural choice because it is an essential part of research with applications in many fields, and there is a network of capable researchers in Africa generated by sustained efforts over the past 10 years.

The U.S.-Africa Initiative in Electronic Structure is supported by of the Innovation Fund of the American Physical Society.

## Recent News

Deadline for ASESMANET is May 15, 2022

ASESMANET opens a call for scientists based in Africa that want to participate and present their research at the Psi-k conference (August 2022 in Lausanne, Switzerland) which usually takes place every 5 years. This call is supported by the Centre Européen de Calcul Atomique et Moléculaire (CECAM), the Psi-k network, the National Centre for Computational Design and Discovery of Novel Materials MARVEL funded by the Swiss National Science Foundation, and by the Office of External Activities (OEA) of the Abdus Salam International Centre for Theoretical Physics (ICTP). Women are particularly encouraged to apply. For more details email asesmanet@eaifr.org or join the USAfrI Slack Channel.

April 30, 2022

The 2022 Workshop on Recent Developments in Electronic Structure will be a hybrid event, held June 1-3, 2022. To register and to see the program, visit the ES22 website.

# The future is very bright

- 2nd decadal plan 2020-2030
- New administrative hub ICTP-EAIFR in Kigali, Rwanda
- ASESMANET

- Many, many exciting success stories

# My thoughts about the future

- Plan for 2025, 2027 and 2029
  - Involve more younger folk in the organisation of ASESMA
  - From Africa and internationally
- Market the success stories of ASESMA more extensively to a global audience
- Train the future African trainers
  - ASESMA already has a number of successful alumni
- Participants need to learn the fundamentals behind the codes
  - Education is important
  - Theory and algorithms
  - Code development; make small modifications to the codes
  - Don’t simply use QE as a black box

# Participants need to

- Be productive with their research
- Drive intra-African collaborations
- Grow international cooperation

- Publish your work
- Present your work at Conferences
  - Hybrid participation is more possible now!

# Apologies

## - I am not involved much in ASESMA anymore

- Vice President IUPAP (Membership and Development)
- I led the incorporation of Ukraine into IUPAP
- New members in Jordan, Egypt, Uruguay, Bulgaria
- I proposed a new category of membership
  - Associate Territorial Member
  - Working with Nepal
- Engaging with Pacific Island nations
  - This region will be disproportionately affected by climate change
- Chair WG Physics and the Green Economy

**IUPAP resolution regarding international conferences in this time**

IUPAP, during the darkest days of the cold war, apartheid and many other difficult political eras over the past 100 years, has always been able to do two things with care and responsibility:

i) Kept open the channels for scientific cooperation across all political and other divides in the hope and expectation that enhanced scientific collaborations are an important means to develop improved understandings between different peoples that contributes to world peace, and

ii) Expressed its concerns about any activity or intervention, including war, that impacts negatively on our ability to engage scientifically on a global scale and hence impacting negatively on (i) above.

IUPAP has issued its statement on the Russian invasion of Ukraine (https://iupap.org/2022/03/01/iupap-statement-on-the-events-occurring-in-ukraine-2022-03-01/) in accordance with (ii) above.

It will be inappropriate for IUPAP to bar any scientist, especially from a member nation, from any scientific activity in accordance with (i) above. So long as the work upholds the ethics and principles of science in its highest ideals, for example, does not contribute to weapons capabilities, IUPAP can see no reason to disallow Russian scientist participation in the affairs of the Union.

**The IUPAP Executive Council**

# Consider …..

- The pursuit of excellence in physics and development of physics on a global scale must go hand-in-hand
  - Focus on excellence, no compromises on international quality
  - A basis of people and societal development

A journey of a thousand miles starts with a single step

But you've got to take that first step. Doing nothing is not an option.

Thank you, Richard!

You've touched the lives of so many of us in so many different ways!