East African Institute for Fundamental Research (EAIFR)

United Nations
Educational, Scientific and
Cultural Organization

ICTP - East African Institute
for Fundamental Research
under the auspices of UNESCO

The Abdus Salam
International Centre
for Theoretical Physics

Republic of Rwanda
Ministry of Education

...Research and Discoveries for African Development and Advancement (RADADA)

Science for African Development and Advancement

Omololu AKIN-OJO

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...Research and Discoveries for African Development and Advancement
(RADADA)

Physics for African Development

Omololu AKIN-OJO

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UNIVERSITY of RWANDA

...Research and Discoveries for African Development and Advancement
(RADADA)

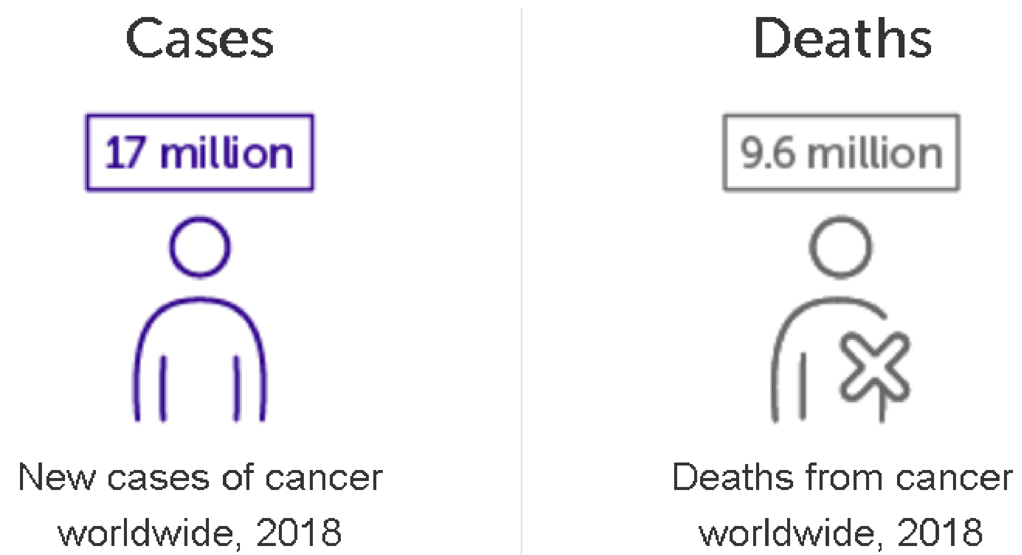
Many Problems in the World

* Food security
* Defense
* Health
* Education
* Energy
* Clean Water
* Mechanization/Automation
* Etc

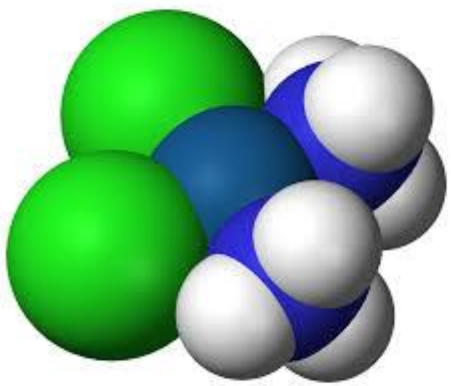
Pick Some and Tackle them

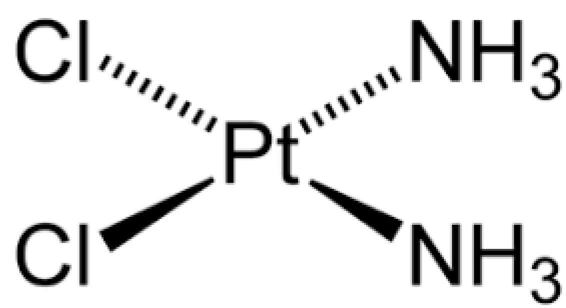
Addressing Problems [in Africa]

Tackling Cancer by "Delivering CISPLATIN"



https://www.cancerresearchuk.org/health-professional/cancer-statistics/worldwide-cancer





...Research and Discoveries for African Development and Advancement (RADADA)

Addressing Problems [in Africa]

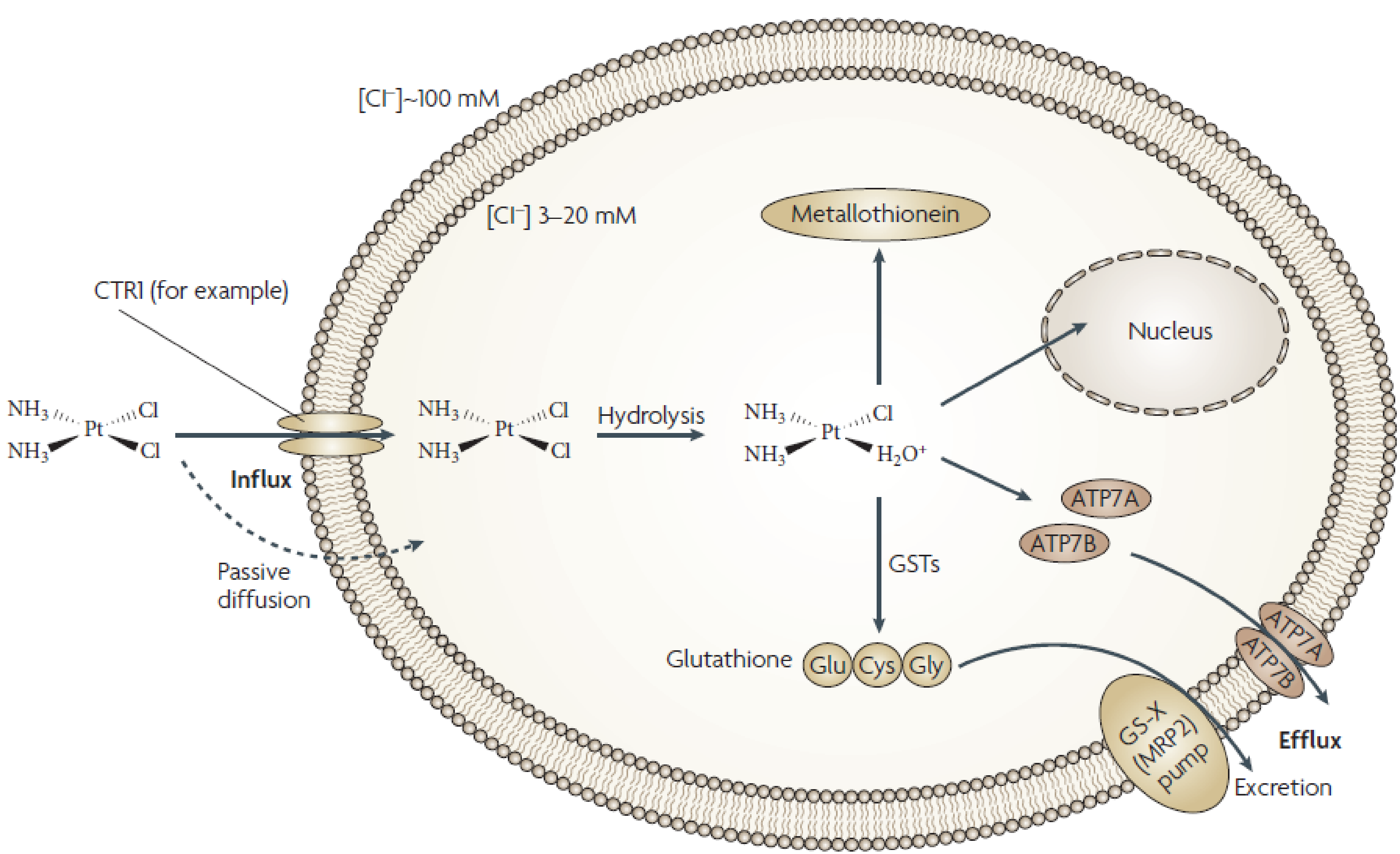


Figure 1 | **Tumour resistance to cisplatin and carboplatin mediated by inadequate levels of platinum reaching target DNA.** Platinum might enter cells using either transporters — a significant one being the copper transporter CTR1

(Image from: Nature Reviews Cancer: L. Kelland (2007))

…Research and Discoveries for African Development and Advancement (RADADA)

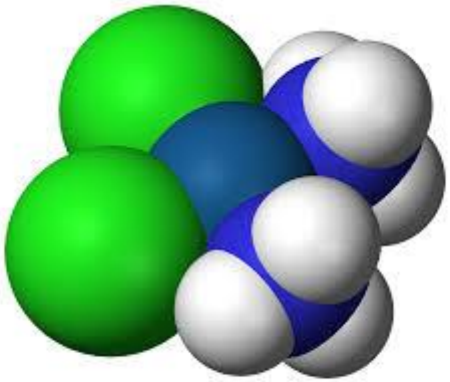
Addressing Problems [in Africa]

Tackling Cancer by "Delivering CISPLATIN"

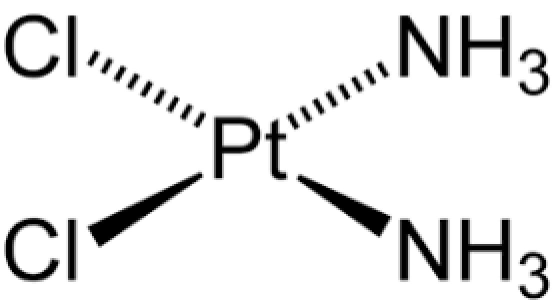
MOLECULAR DYNAMICS SIMULATION OF TRANSPORT OF ENCAPSULATED DRUG THROUGH A LIPID BILAYER

MASTERS DEGREE IN THEORETICAL PHYSICS

By



Ibrahim Buba Garba



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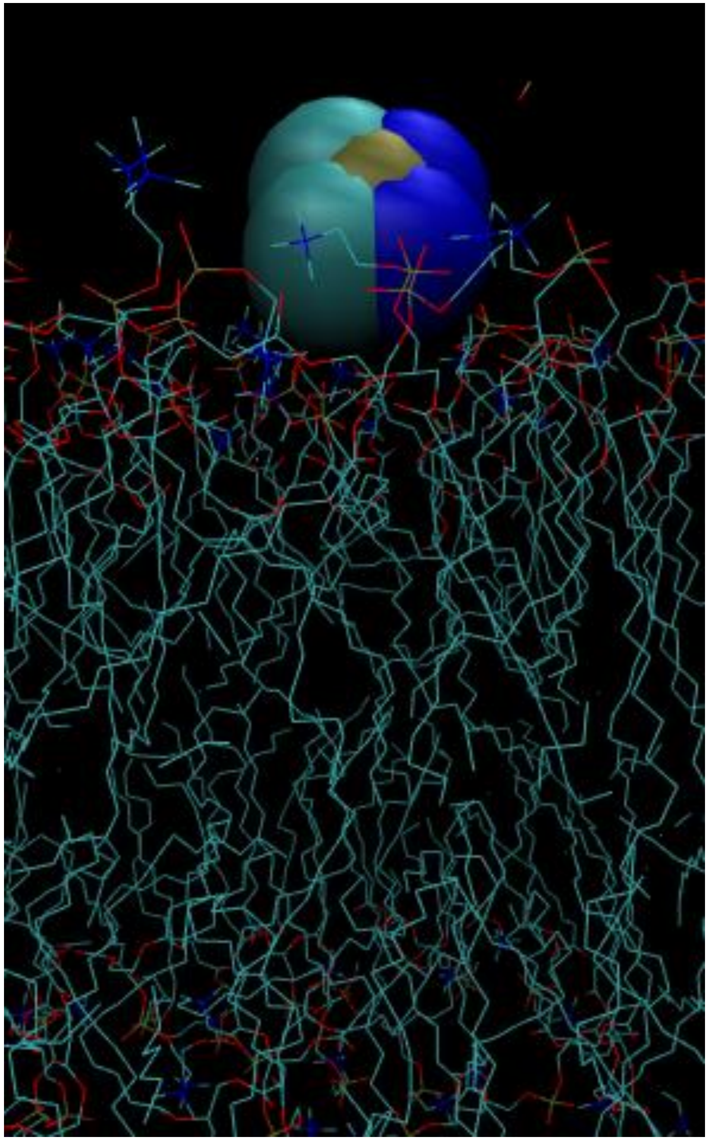
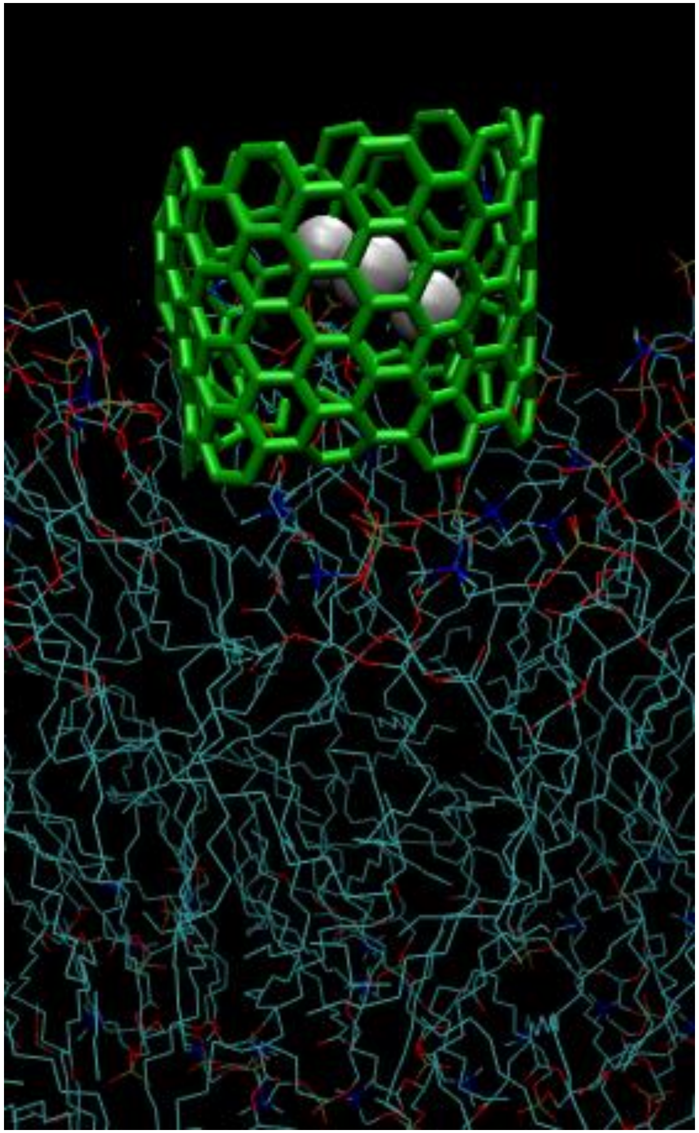
Addressing Problems [in Africa]





...Research and Discoveries for African Development and Advancement (RADADA)

Molecular Dynamics (MD) simulations

$$\vec{F} = m\vec{a} \qquad\qquad m\vec{a} = \vec{F}$$

$$m\frac{d^2x}{dt^2} = -\nabla E$$

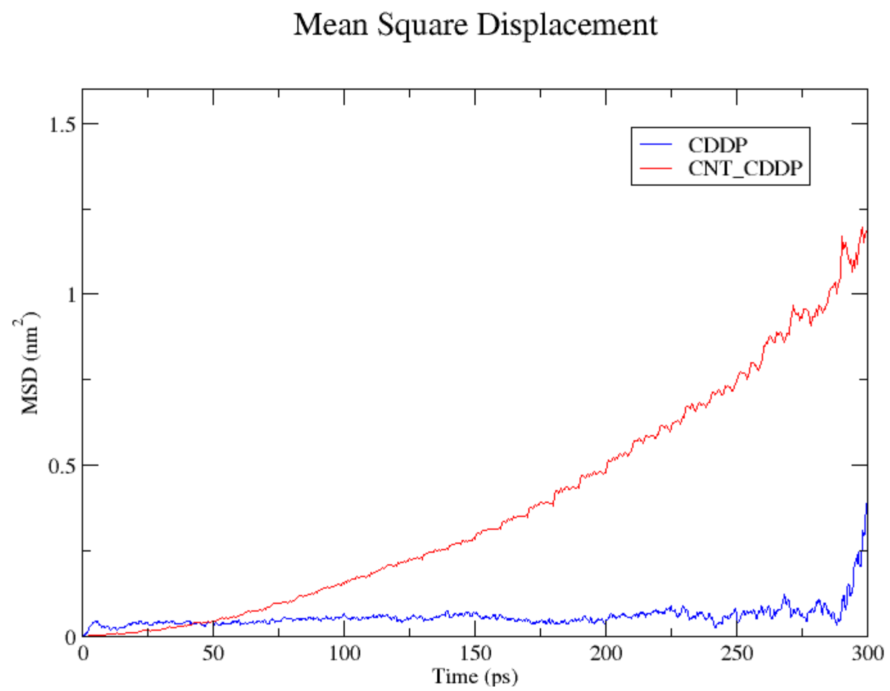
$$m_i\frac{d^2\vec{r}_i}{dt^2} = -\nabla_i E(\vec{r}_1, \ldots, \vec{r}_N)$$

$$m_1\frac{d^2x_1}{dt^2} = -\frac{\partial E}{\partial x_1} \qquad\qquad m_N\frac{d^2x_N}{dt^2} = -\frac{\partial E}{\partial x_N}$$

$$m_1\frac{d^2y_1}{dt^2} = -\frac{\partial E}{\partial y_1} \qquad\qquad m_N\frac{d^2y_N}{dt^2} = -\frac{\partial E}{\partial y_N}$$

$$m_1\frac{d^2z_1}{dt^2} = -\frac{\partial E}{\partial z_1} \qquad\qquad m_N\frac{d^2z_N}{dt^2} = -\frac{\partial E}{\partial z_N}$$

Addressing Problems [in Africa]

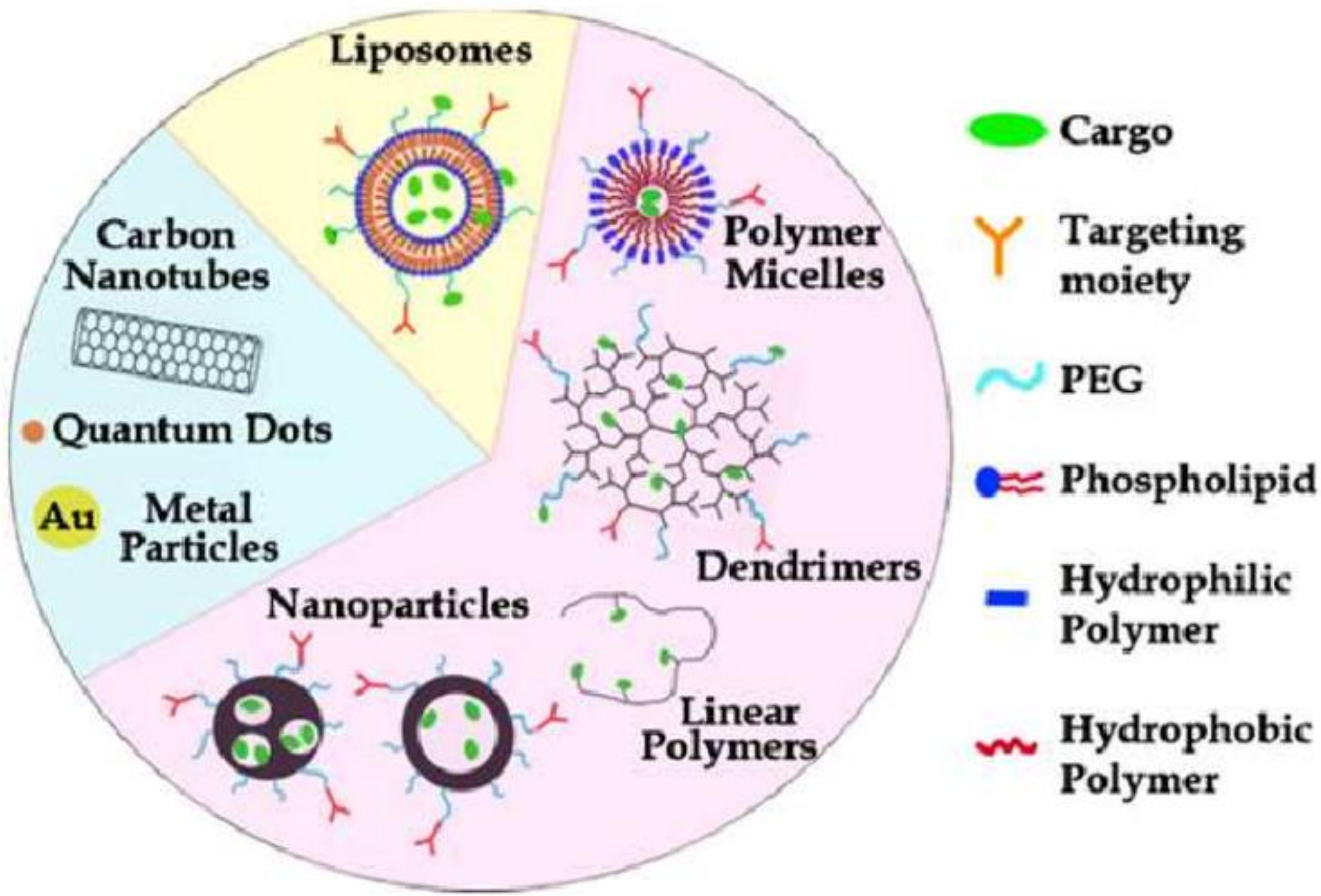


$$D_A = \lim_{t \longrightarrow \infty} \frac{1}{2td} \langle |\mathbf{r}_i(t) - \mathbf{r}_i(0)|^2 \rangle_{i \in A}$$

System	$D_s(10^{-5}\ cm^2 s^{-1})$	Error Estimate
CDDP	0.2196	0.2591
CNT-CDDP	0.6149	0.1336

...Research and Discoveries for African Development and Advancement (RADADA)

Nanotech for Drug Delivery. Cancer.



Hsu, Janet and S. Muro. "Nanomedicine and Drug Delivery Strategies for Treatment of Genetic Diseases." (2011).

…Research and Discoveries for African Development and Advancement (RADADA)

Nanotech for Drug Delivery. Cancer.

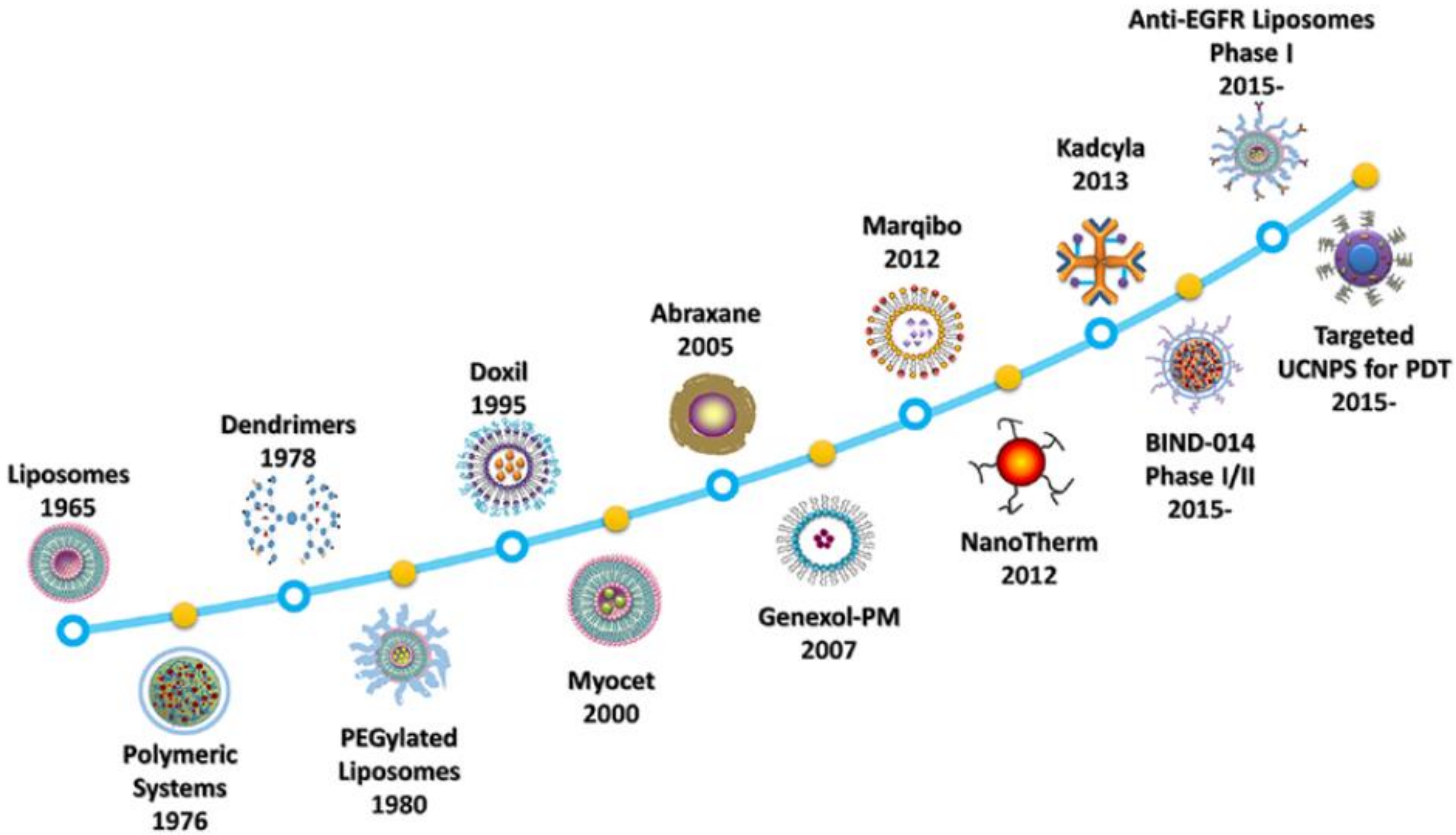


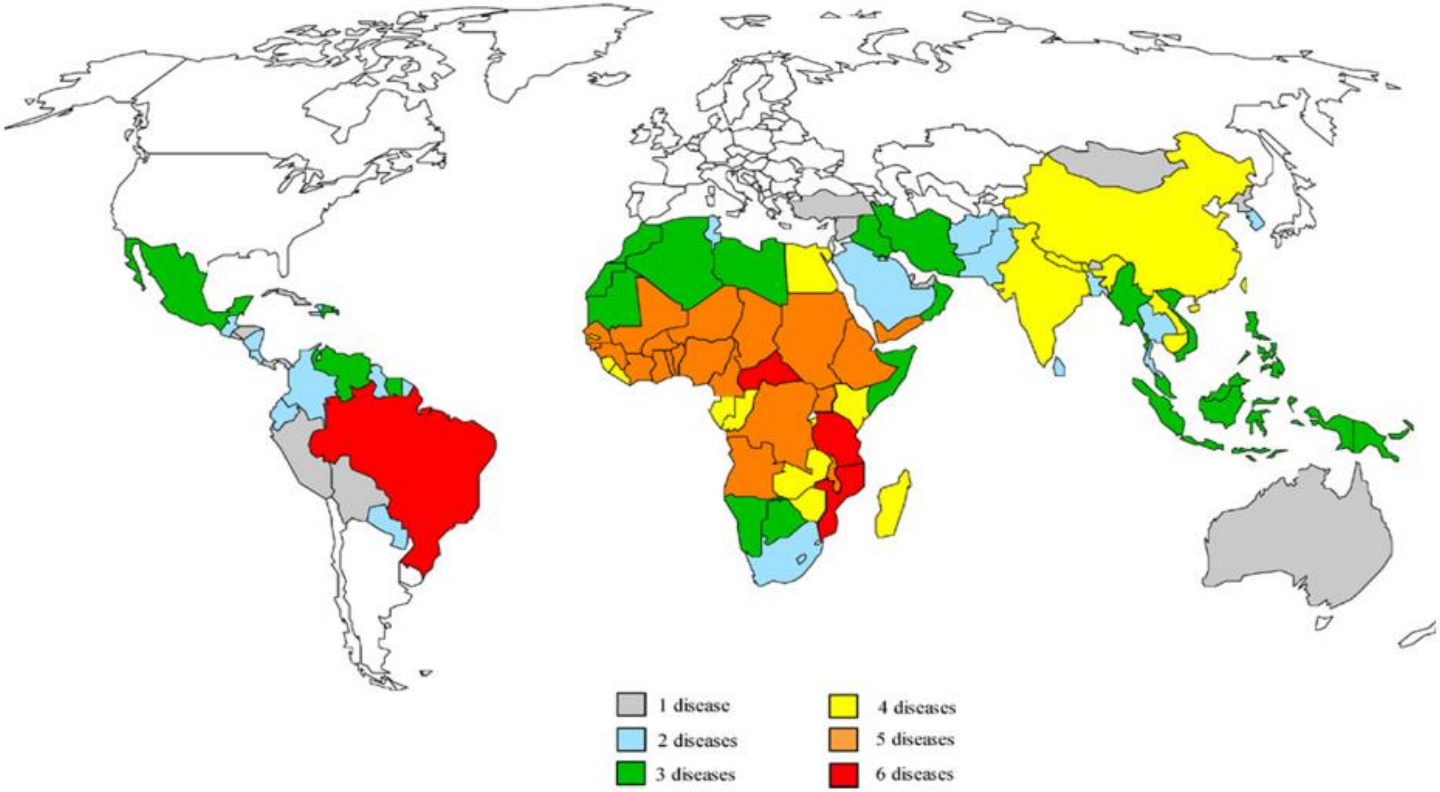
Figure 1. Timeline of the development of nanomedicines. Liposomes (5), polymeric systems (151), dendrimers (152), and PEGylated liposomes (153) were developed as nanodrug carriers in the early phase of discovery (before 1995). Doxil (doxorubicin) was the first FDA-approved liposome for use in cancer (154).

Addressing Problems in Africa (Future)

"Neglected Tropical Diseases"

Global distribution of NTDs

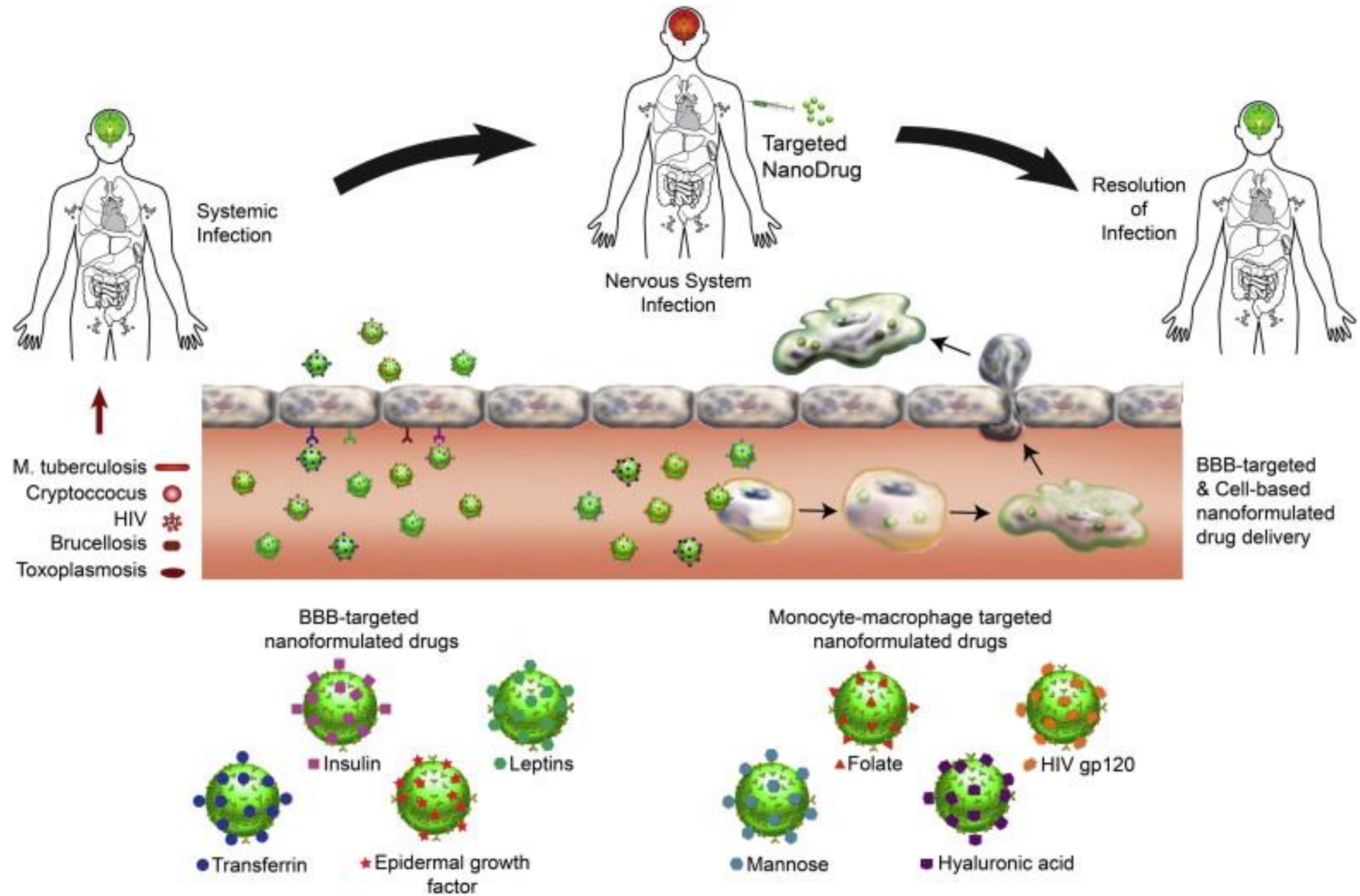
Approximately 1 billion people are affected by more than one of NTDs



Source: Savioli, L. (2010). *Neglected Tropical Diseases (NTDs): Yesterday's drain, tomorrow's gain for global health*. Retrieved July 27, 2010, from http://ntd.rti.org/publications/index.cfm?fuseaction=throwpub&ID=220

...Research and Discoveries for African Development and Advancement (RADADA)

Nanotech for Drug Delivery. IDs.



Gendelman HE, et al, Nanoneuromedicines for degenerative, inflammatory, and infectious nervous system diseases. Nanomedicine:
NBM 2015;11:751-767, http://dx.doi.org/10.1016/j.nano.2014.12.014

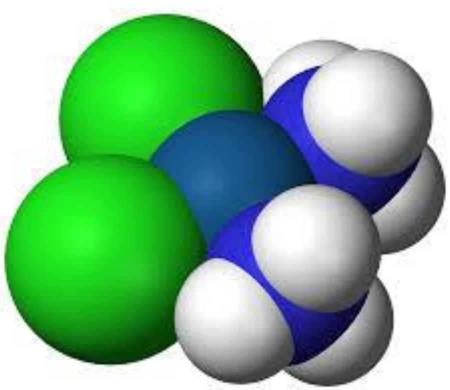
Addressing Problems [in Africa]

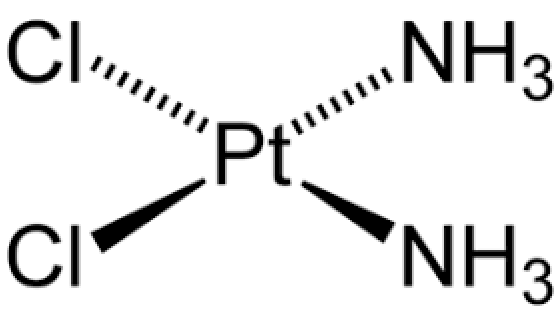
Molecular Dynamics Simulations of the Interaction of Cisplatin with DNA, RNA and Proteins

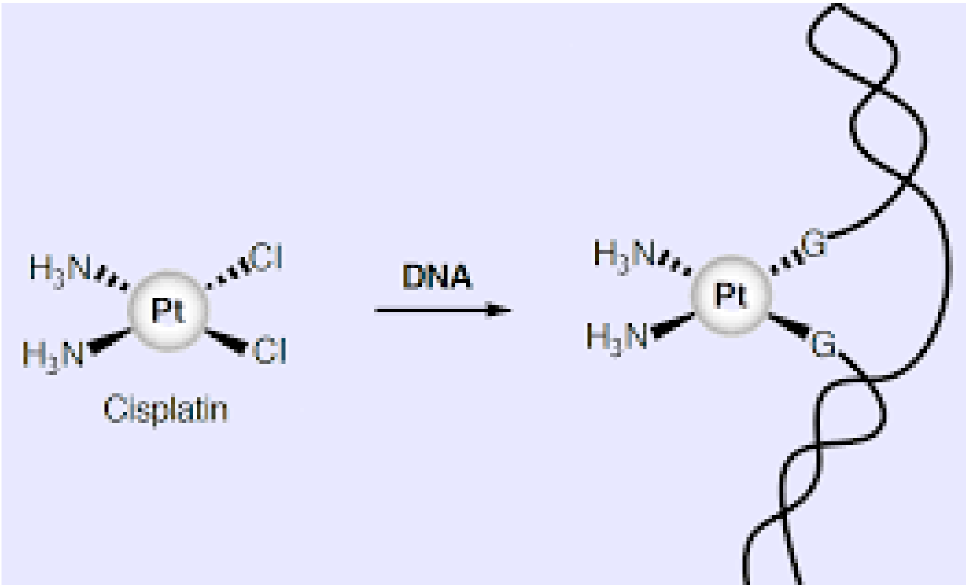
Adebayo Oluseun ADENIYI[1], Omololu AKIN-OJO[2]

[1] Department of Theoretical and Applied Physics, African University of Science and Technology, Abuja, Nigeria
[2] East African Institute for Fundamental Research, Rwanda

"CISPLATIN"







...Research and Discoveries for African Development and Advancement (RADADA)

Addressing Problems in Africa (Future)

"Neglected Tropical Diseases"

Global distribution of NTDs

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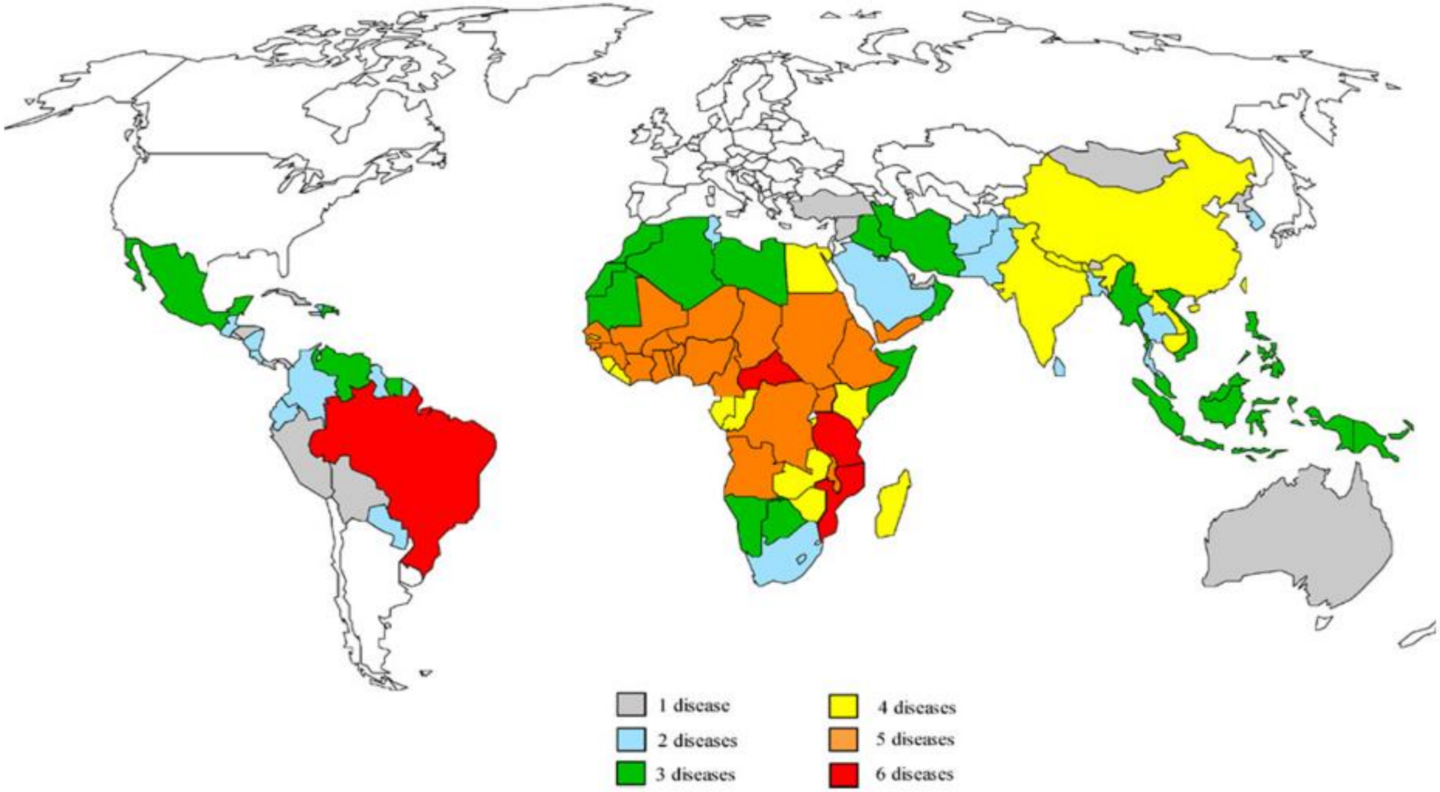

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…Research and Discoveries for African Development and Advancement (RADADA)

Many Problems in the World

* Food security
* Defense
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* Clean Water
* Mechanization/Automation
* Etc

Pick Some and Tackle them

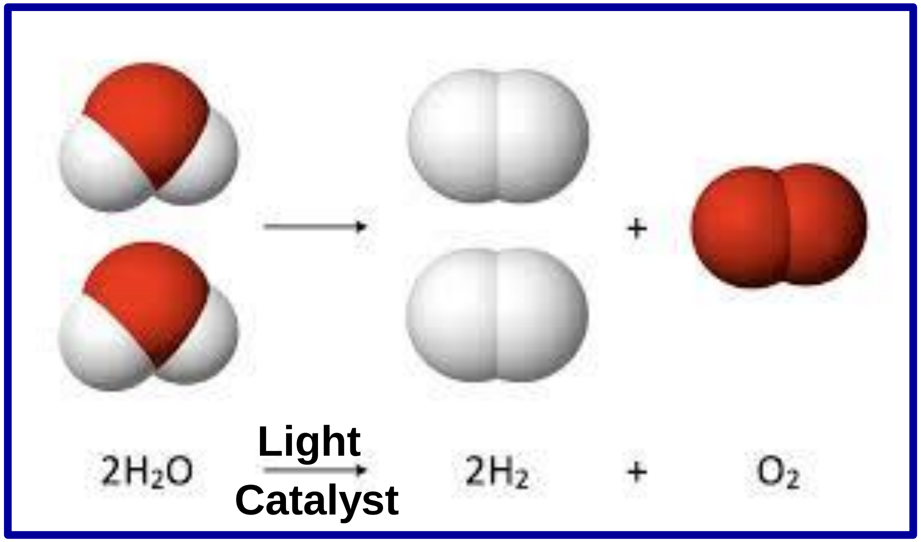
Addressing Problems in Africa
(Hydrogen gas → Cooking Fuel?)

<u>Cooking with biomass</u>

* 3B people worldwide
* > 3.8 m deaths yearly – health related problems
* Robs girls of school time
* Potential solution: Clean Hydrogen from Water

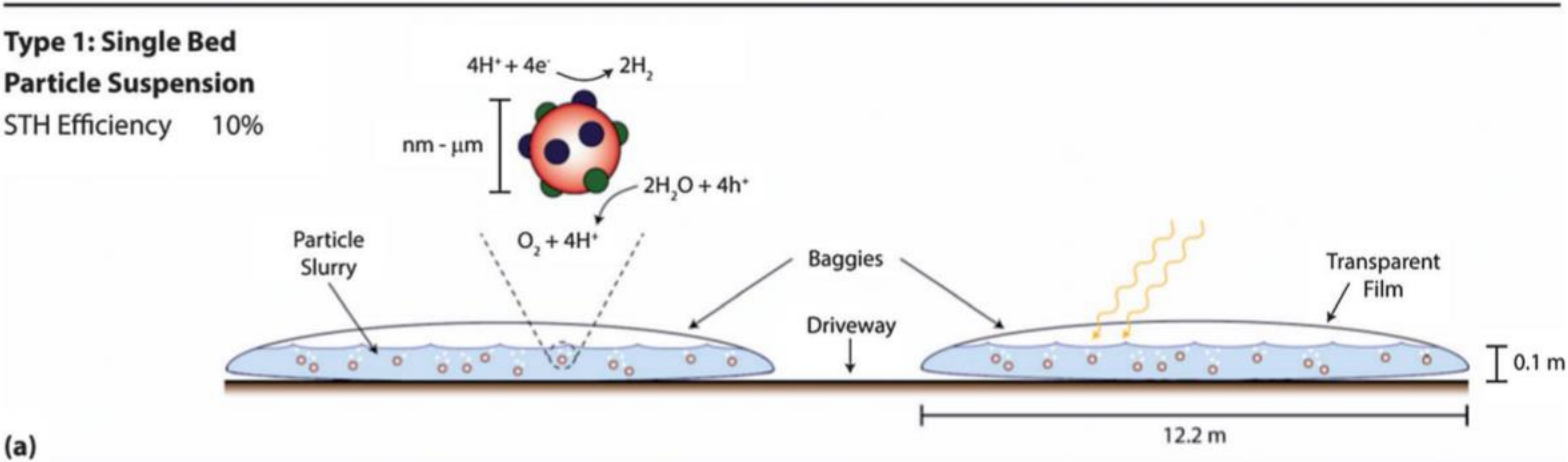
...Research and Discoveries for African Development and Advancement (RADADA)

Addressing Problems in Africa
(Hydrogen: Water Splitting)



Design Cheap Catalysts!
Solve Energy [and Water] Problems!

Addressing Problems [in Africa] Catalysts for Hydrogen Production



(Image from: Pinaud et. al., Energy Environ. Sci., 2013, 6, 1983–2002)

...Research and Discoveries for African Development and Advancement (RADADA)

Addressing Problems in Africa
(Water Splitting: Design Catalyst)

1. From Data Base Choose Direct Band Gap Materials with 1.23 < BG < 1.8 – 2.2 eV

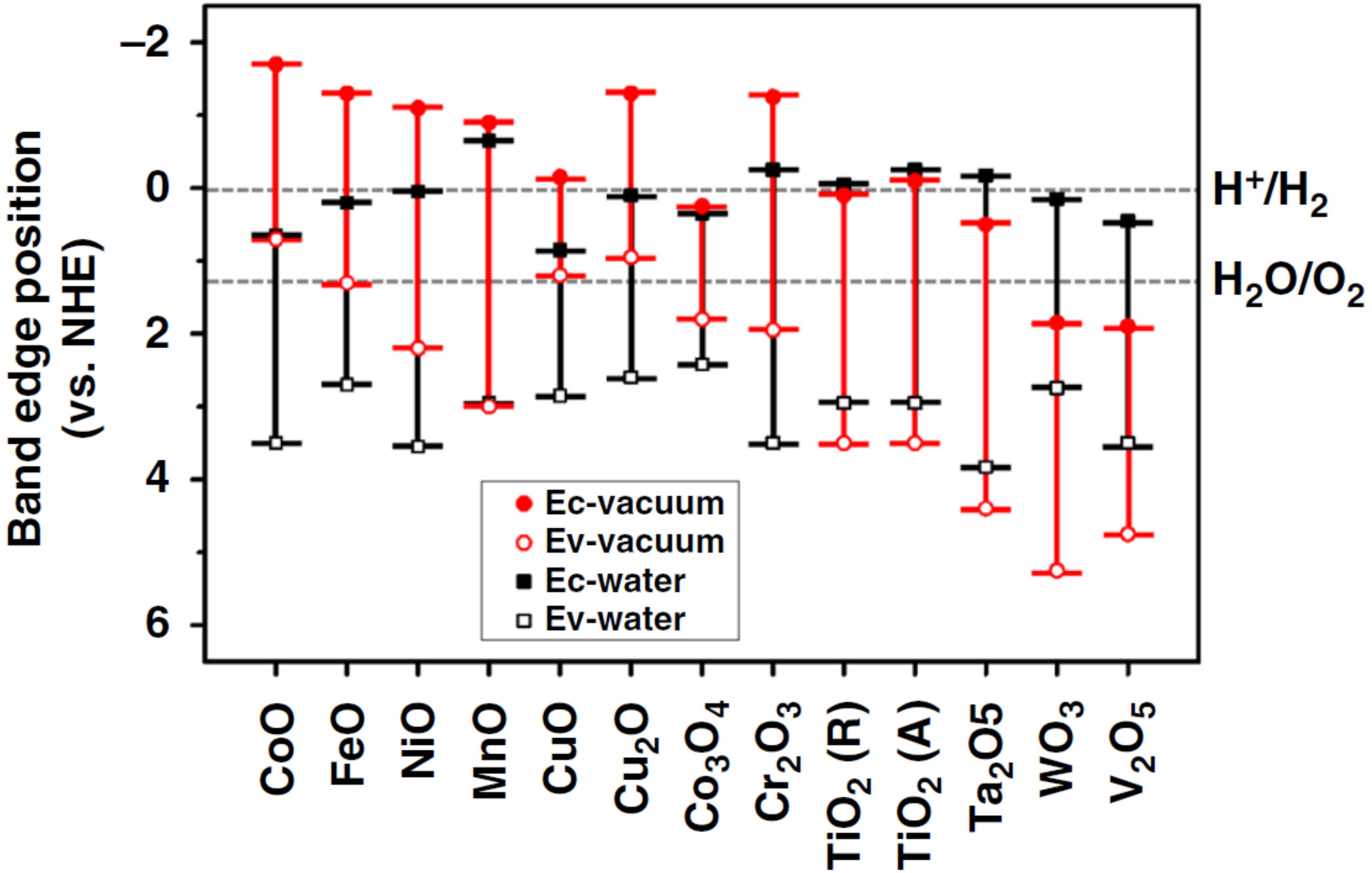
2. Use Empirical Model(s) or Machine Learning to Determine Absolute Band Edge Positions of Catalysts **in Water**

3. Corrosion Effects?

4. STH Efficiency =?

E.g., See the paper by Dabo et. al.:
Energy Environ. Sci., 2021,**14**, 2335-2348

Addressing Problems in Africa
(Hydrogen: Water Splitting)



Park, KW., Kolpak, A.M. Optimal methodology for explicit solvation prediction of band edges of transition metal oxide photocatalysts. *Commun Chem* **2,** 79 (2019). https://doi.org/10.1038/s42004-019-0179-3

…Research and Discoveries for African Development and Advancement

Many Problems in the World

* Food security
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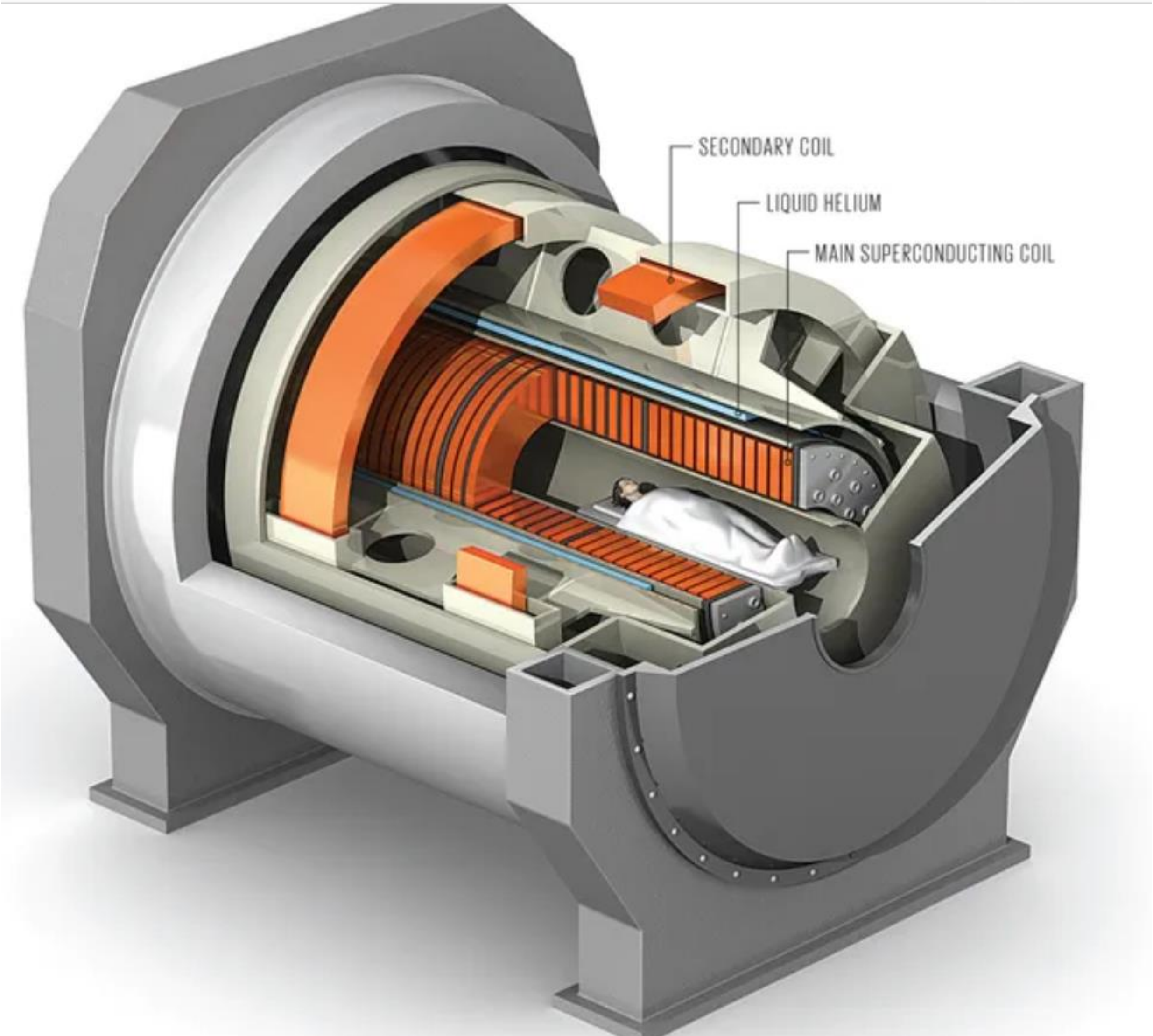
Pick Some and Tackle them

Addressing Problems [in Africa]
(Room Temp Superconductors for MRI)



https://spectrum.ieee.org/the-worlds-most-powerful-mri-takes-shape
Picture Credit: Emily Cooper

Machine Learning the Superconducting Critical Temperatures of Metals

Firas SHUAIB
Omololu AKIN-OJO

ICTP-EAIFR

SUPERCONDUCTIVITY

Zero Resistivity (K.Onnes, 1911)
Perfect Diamagnetism (Meissner-Ochsenfeld, 1933)

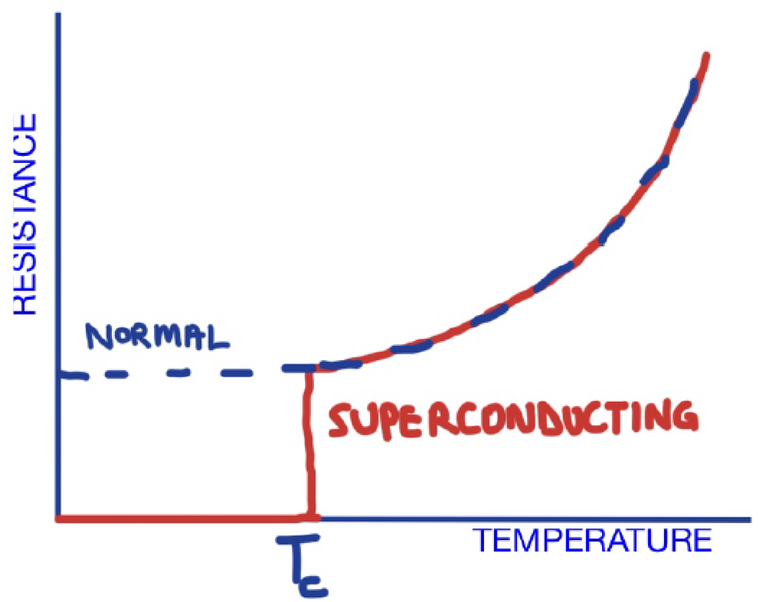


Figure : Zero Resistance

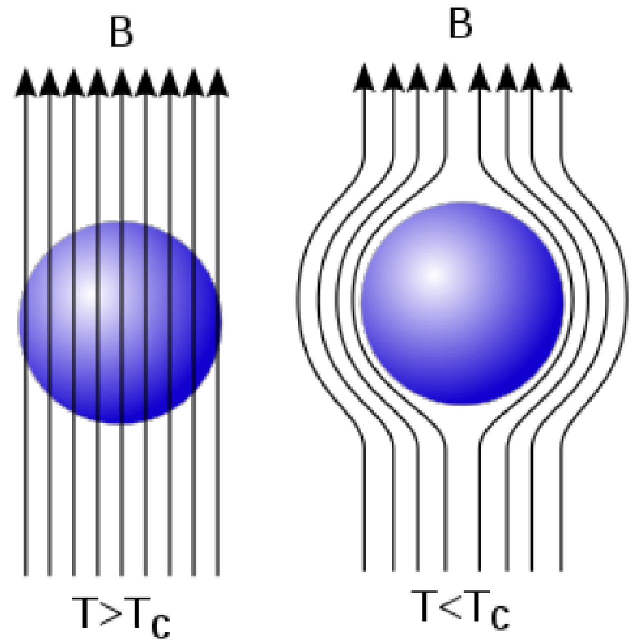


Figure : Perfect Diamagnetism

...Research and Discoveries for African Development and Advancement (RADADA)

- Apply **ML to predict** T_c
  (Focus on el-phonon superconductors).
  - Use data from the AFLOW database `http://aflow.org/search/thermal-lib.php`.
  - Use data from the SuperCond database.

- Apply the best model to **search** for potential new superconductors in the Inorganic Crystallographic Structure Database **(ICSD)**.

A Main Question

Which atomistic **properties/descriptors** make a material superconducting?
BCS: $T_c = 1.14\theta_D \exp[-1/\lambda]$

$$\lambda = 2\int \alpha^2 F(w)\frac{dw}{w} \simeq N(0)V \quad (1)$$

$$\theta_D = \frac{3nhN_A\rho^{1/3}}{4\pi k_B M} v_m \quad (2)$$

Where:
$F(w) \equiv$ phonon DOS. $M \equiv$ Atomic weight.
$n \equiv$ Number of atoms per primitive unit cell.
$v_m \equiv$ Averaged wave velocity. $\rho \equiv$ Mass density So:

- Electronic band structure: N(0)
- Features of phonon spectrum e.g Debye temperature θ_D.
- El-phonon coupling constant λ.

Methodology

- Targets:
  - θ_D from **AFLOW** database $\simeq$ 5200.
  - $N(0)$ from calculated DOS in **AFLOW** $\simeq$ 13600.
  - T_c for metals ($N(0) \neq 0$) from **SuperCond** database $\simeq$ 4000.
- Descriptors
  - Obtained from the chemical formula of the compound using (Materials Agnostic Platform for Informatics and Exploration) **MAGPIE**.
- ML Models Used (in Scikitlearn)
  - Linear Regression LR.
  - Ridge Regression RR.
  - Random forest RF.

Descriptors (from MAGPIE)

$$\theta_D = \theta_D(\text{desc}_1, \text{desc}_2, \ldots)$$

Chemical Formula

$\longrightarrow$ Min, Max, Mode, Mean, Avg_Dev, of atomic weights.

$\longrightarrow$ Min, Max, Mode, Mean, Avg_Dev, of electronegativities.

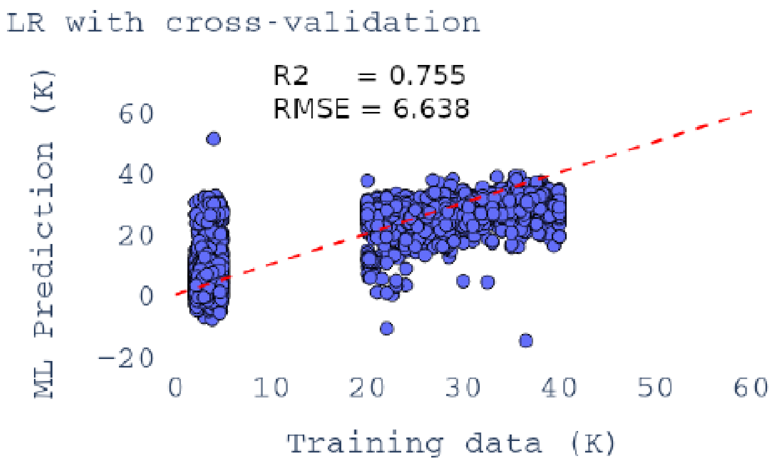
$\longrightarrow$ Estimated melting temperature.

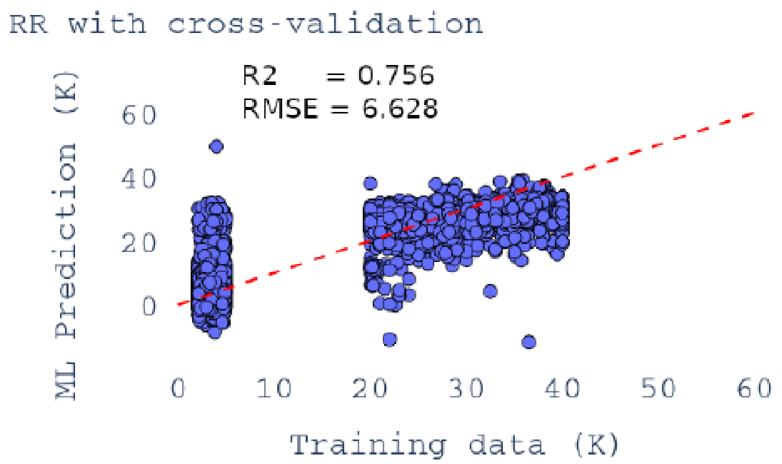
$\longrightarrow$ $\vdots$

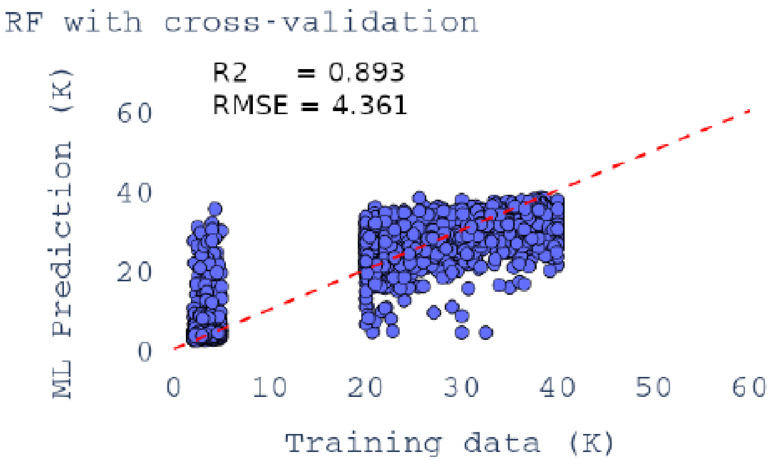
$\longrightarrow$ etc

132 descriptors in all.

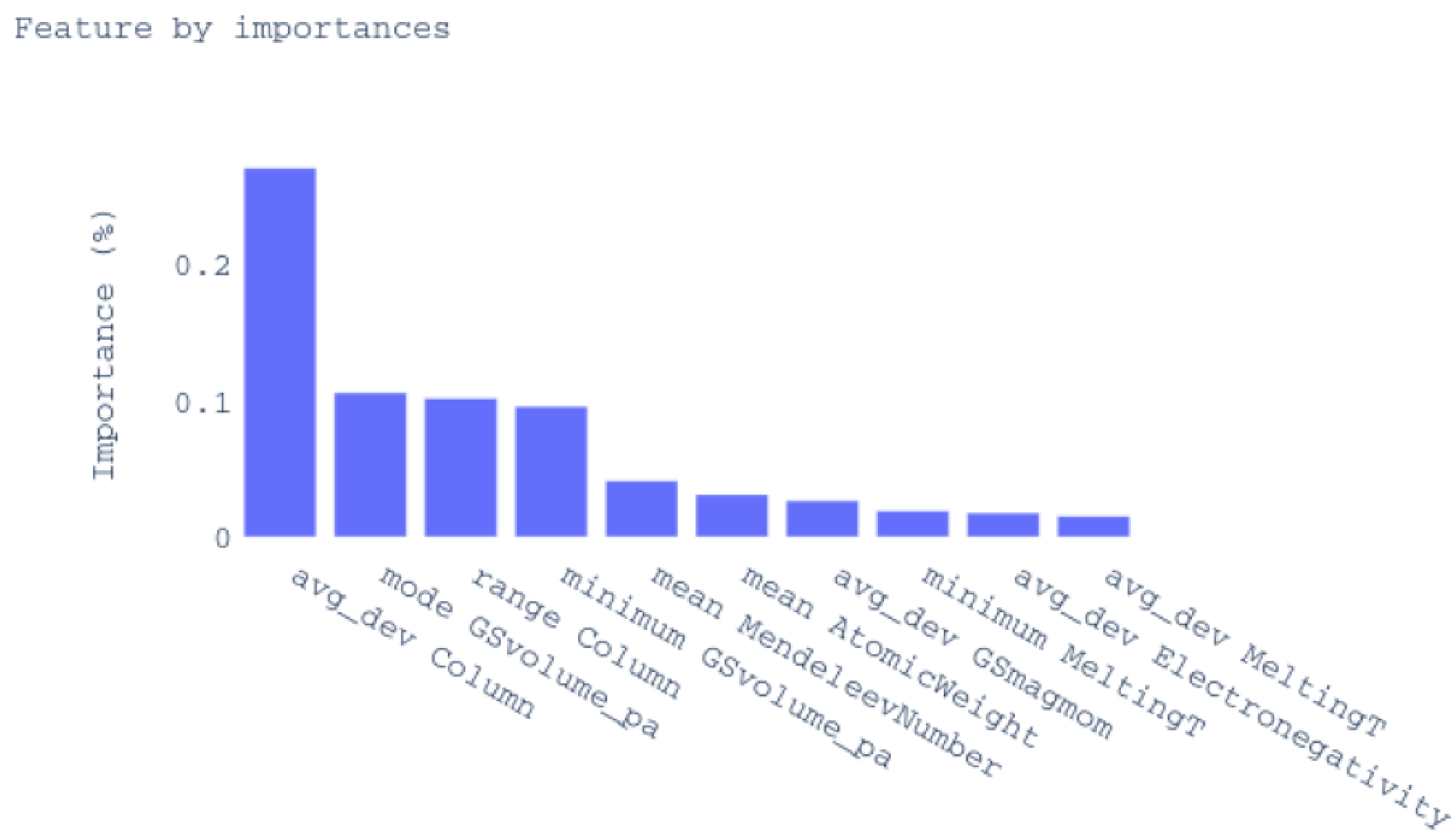
Result: Training T_c (with cross-validation)







Result: The most important features used by RF model for T_c



...Research and Discoveries for African Development and Advancement (RADADA)

Compare the RF prediction of T_c to the experimental value for top ten compounds.

Training data top ten T_c List		
Compound Name	T_c	Predict T_c
La2Cu0.965V0.035O4.045	40	39.564
La2Cu0.975V0.025O4.032	40	39.366
La2Cu0.955V0.045O4.056	40	39.197
La1.98Sr0.02Cu1O4.09	40	39.074
La0.5Y0.5Fe1As1O0.6	39.3	38.345
La1.828Sr0.172Cu1O4	39.35	38.173
Mg0.9Zn0.1B2	38.4	38.139
Mg0.996Cu0.004B2	38.11	37.918
Y1Ba2Cu3.94Zn0.06O8	39.6	36.323
Eu1.3Ba1.7Cu3O7.15	39.5	36.098

Search for potential new superconductors in the Inorganic Crystallographic Structure Database (ICSD)

Based on the experience from previous data:

ICSD top ten T_c List			
Compound Name	θ_D	$N(0)$	T_c
B2Mg1	623.464	1.759	38.072
Ba2Cu4O8Y1	193.339	2.053	34.953
Cu1O2Sr1	203.814	1.353	34.527
Ba2Cu3Eu1O7	175.297	3.339	34.514
Cu2Gd1O8Ru1Sr2	182.628	5.058	34.328
Ba6Ca6Cu9O29Tl5	165.822	8.015	34.107
Ba2Cu4Ho1O8	179.893	11.999	33.869
Ba2Cu4Er1O8	181.338	3.493	33.505
Ba2Cu1O5Tl1	144.462	5.354	32.753
Ca1Cu1O2	231.596	1.225	32.629

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