Environmental Science

Unit –IV Research, and Policies related to Environment

(Recent research on detection of water and air pollution using various nanostructures, Environment protection Act, national forest policies, wildlife protection act.)
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By
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विश्वजीवनामृतं ज्ञानम्

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5 survival needs of humans:

The truth is, there are five basic needs;

Clean **Air**,

Water,

Nutrients,

Shelter and

Sleep.

Beyond our health, the simple fact is that our entire society is based primarily on the existence and leveraging of these five factors.

They are the basis for concepts like family, wealth, health and, at times, governments.

Challenges of World

Pollution

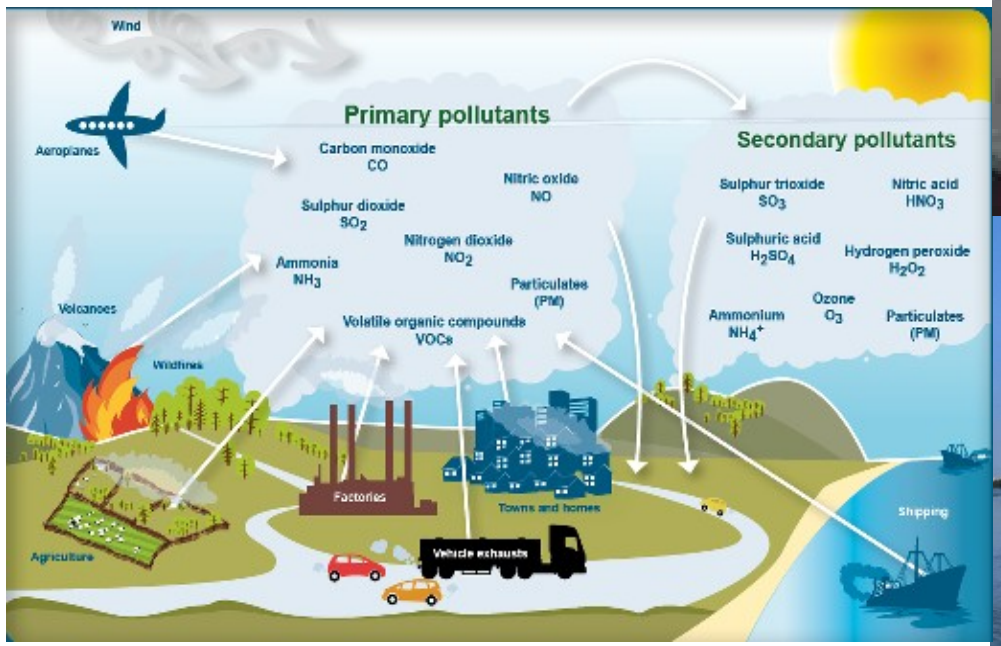
Pollution is Hazardous to Environment

"Any undesirable change in the physical, chemical, biological characteristics of any component of the environment which can cause harm to life and property"

1 Air pollution | 2 Water pollution | 3 Soil pollution | 4 Noise pollution

Challenges and Opportunities: Air and Water Pollution

The harmful pollutants responsible for polluting the environment are: Nitrogen oxide | Sulphur oxide | Mercury | Particulate matter | Chlorofluorocarbon | Volatile organic compounds



Air pollution in India is responsible for 12.5 percent of all deaths in the country, according to the State of **India's** Environment (SoE) report, **2019**. 8.5 out of every 10,000 children in **India** die before they turn five due to poor **air**.

Air pollution

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A study by the Health Effects Institute found that unhealthy levels of PM 2.5 led to roughly 852,000 premature deaths in **China** in 2017.

Latest India Air quality reports on worldmap

India Environment Portal
KNOWLEDGE FOR CHANGE

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2018 world air quality report

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01/03/2019 | *IQAir AirVisual*

India's national capital region (NCR) emerged as the most polluted region in the world in 2018, according to this new report. Gurugram is the worst affected followed by Ghaziabad, Faridabad and Noida are amongst the top six most worst-affected cities.

Delhi has been ranked the most polluted capital in the world, while Gurugram is the most polluted city, according to a Greenpeace report. According to the latest data compiled in the IQ Air Visual 2018 World Air Quality Report and interactive world's most polluted cities ranking, which is prepared in collaboration with Greenpeace Southeast Asia in order to reveal the state of particulate matter (PM2.5) pollution in 2018, Delhi had an average yearly PM2.5 concentration at 113.5 micrograms per cubic metre. The report is based on air quality data collected in 2018 from public monitoring sources, with a special focus on data which has been published in real-time or near real-time.

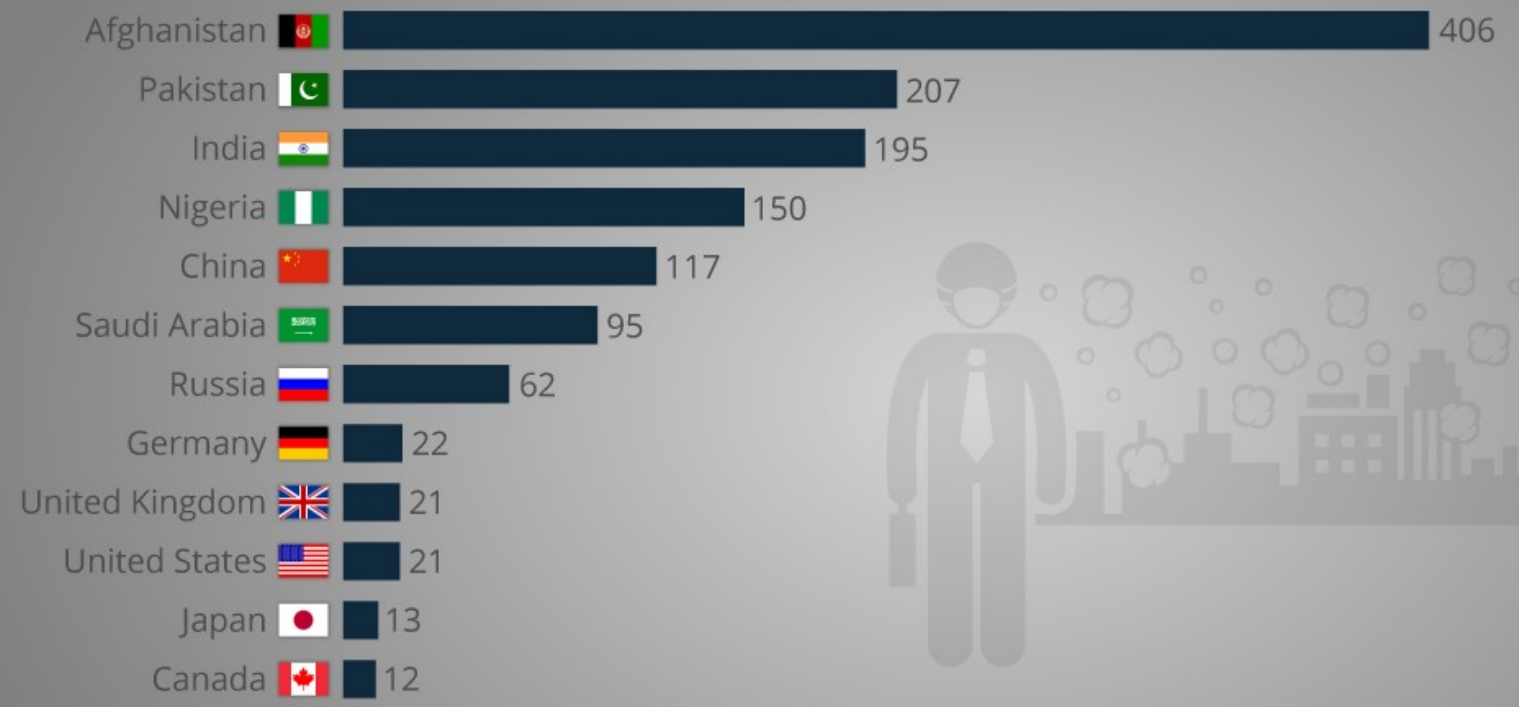
22 out of 30 most polluted cities of the world are from India

13 out of 20 most polluted cities of the world are from India in 2016 WHO report Gwalior in top 3

*http://www.indiaenvironmentportal.org.in/content/461648/2018-world-air-quality-report/

Deaths From Air Pollution Worldwide

Age-standardized deaths per 100,000 people attributable to air pollution (2016)*

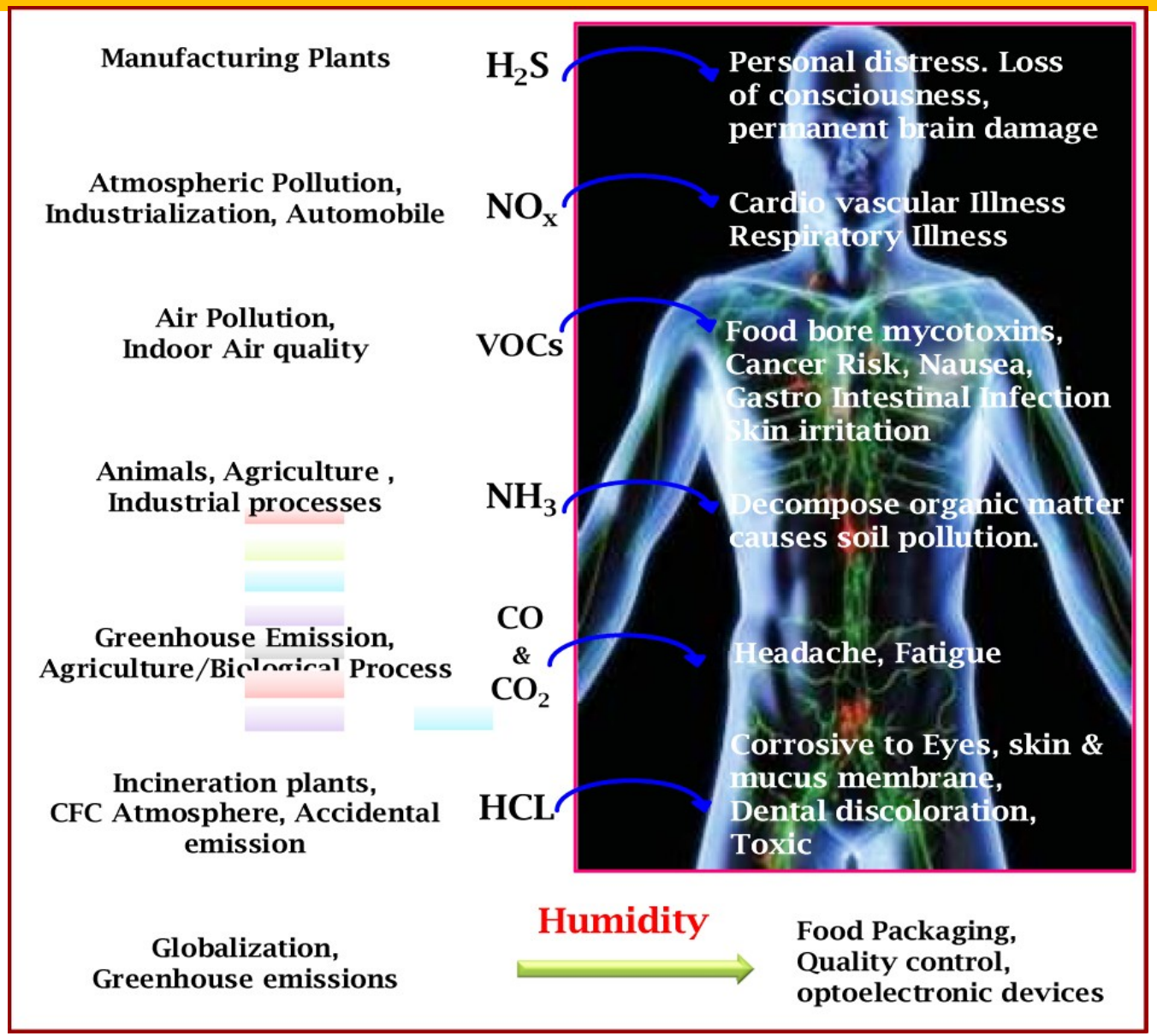


* Selected countries. Age-standardized takes into account deaths per 100,000 people and standardizes based on the age structure of the population. It therefore corrects for population size and age demographics.

@StatistaCharts

Source: Health Effects Institute: State of Global Air 2018

statista


Manufacturing Plants
H_2S
Personal distress. Loss of consciousness, permanent brain damage
Atmospheric Pollution, Industrialization, Automobile
NO_x
Cardio vascular Illness Respiratory Illness
Air Pollution, Indoor Air quality
VOCs
Food bore mycotoxins, Cancer Risk, Nausea, Gastro Intestinal Infection Skin irritation
Animals, Agriculture , Industrial processes
NH_3
Decompose organic matter causes soil pollution.
Greenhouse Emission, Agriculture/Biological Process
CO & CO_2
Headache, Fatigue
Incineration plants, CFC Atmosphere, Accidental emission
HCL
Corrosive to Eyes, skin & mucus membrane, Dental discoloration, Toxic
Humidity
Globalization, Greenhouse emissions
Food Packaging, Quality control, optoelectronic devices

WATER POLLUTION

Water pollution occurs when **harmful pollutants and particulate matter** are introduced into a water body. These contaminants are generally introduced by human activities like improper sewage treatment, oil spills. However, even natural processes such as eutrophication can cause water pollution.

Other significant causes of water pollution include:

- Dumping solid wastes in water bodies
- Disposing untreated industrial sewage into water bodies
- Human and animal wastes
- Agricultural runoff containing pesticides and fertilisers

The effects of water pollution are very pronounced in our environment. Furthermore, toxic chemicals can bioaccumulate in living beings, and these chemicals can travel their way up the food chain, ultimately reaching humans.

WATER

42 rivers have extremely high concentration of neurotoxic heavy metals

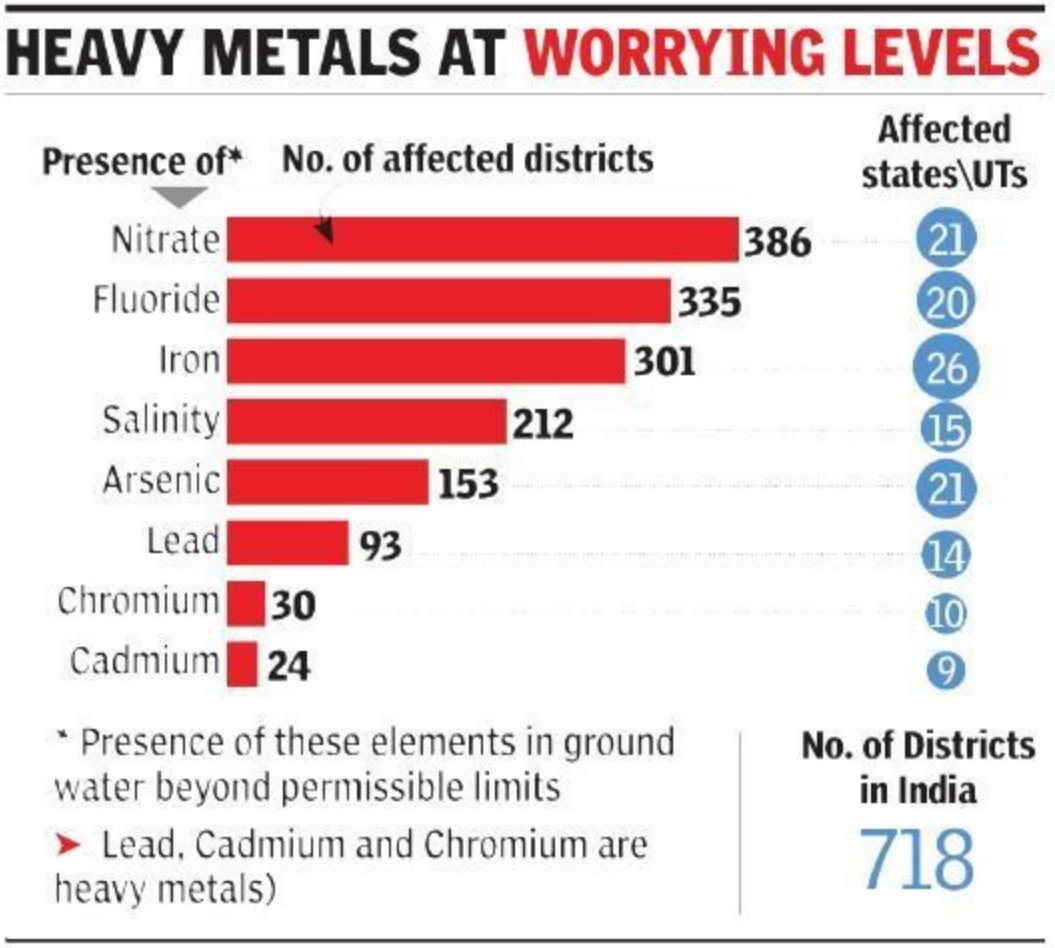
Ganga was found to be polluted with five heavy metals, namely chromium, copper, nickel, lead and iron

By Kiran Pandey, Rajit Sengupta, Isha Bajpai
Published: Tuesday 15 May 2018

Out of Total 400 Rivers

Number of rivers polluted with unacceptable levels of heavy metals

Contaminant	Permissible limit	No of rivers
Lead	10 µg/L	69
Nickel	20 µg/L	25
Iron	300 µg/L	137
Copper	50 µg/L	10
Chromium	50 µg/L	21
Cadmium	3 µg/L	25



Water Pollution

THE TIMES OF INDIA

80% of India's surface water may be polluted, report by international body says

TOI

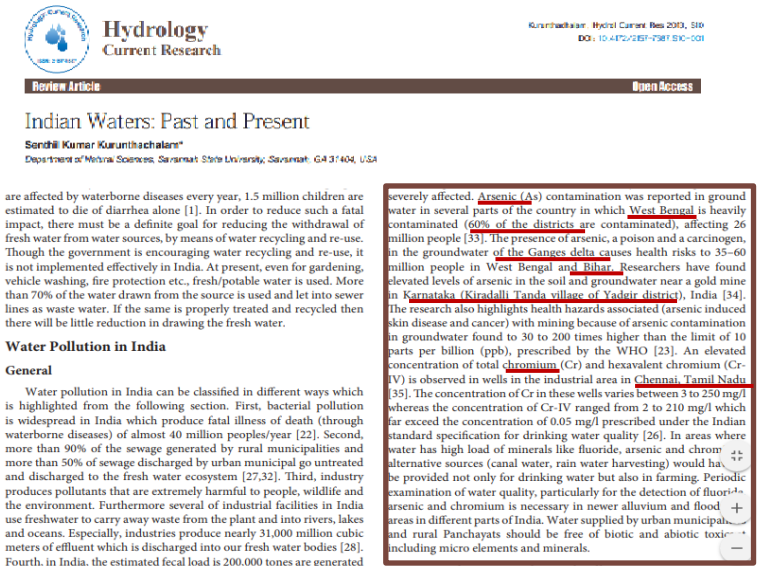
https://timesofindia.indiatimes.com/home/environment/pollution/80-of-Indias-surface-water-may-be-polluted-report-by-international-body-says/articleshow/47848532.cms

Global Ecology and Conservation

Total concentrations and sources of heavy metal pollution in global river and lake water bodies from 1972 to 2017

Qiaoqiao Zhou, Nan Yang, Youzhi Li, Bo Ren, Xiaohui Ding, Hualin Bian, Xin Yao

Abstract: This study collected past sampling data on total concentrations of 12 heavy metals (Cd, Pb, Cr, Hg, Zn, Cu, Ni, Al, Fe, Mn, As, and Co) in surface water bodies, i.e., 168 rivers and 71 lakes, from 1972 to 2017. The intent was to investigate the levels and sources of heavy metal pollution across five decades and five continents. Mean heavy metal concentrations in global river and lake water, and the number of heavy metals with concentrations greater than the published threshold limits as per the standards of both the World Health Organization (WHO) and the United States Environmental Protection Agency (USEPA) were generally lower in the 1970s and 1980s than in the 1990s, 2000s, and 2010s. Over time, heavy metal pollution in surface water has changed from single metal pollution to mixed metal pollution. Heavy metal concentrations in water, and the number of heavy metals with concentrations above the threshold limits for both WHO and USEPA standards were lower in the developed countries of Europe and North America, and higher in the developing countries of Africa, Asia, and South America. Over time, the main sources of metal pollution have changed from mining and manufacturing to rock weathering and waste discharge. The main metal sources differed across the five continents, with fertilizer and pesticide use, along with rock weathering, being dominant in Africa. Mining and manufacturing, along with rock weathering, were dominant in Asia and Europe. Mining and manufacturing, along with fertilizer and pesticide use, were dominant sources in North America, while four sources



Hydrology Current Research

Review Article — Open Access

Indian Waters: Past and Present

Senthil Kumar Kurunthachalam*

Department of Natural Sciences, Savannah State University, Savannah, GA 31404, USA

are affected by waterborne diseases every year, 1.5 million children are estimated to die of diarrhea alone [1]. In order to reduce such a fatal impact, there must be a definite goal for reducing the withdrawal of fresh water from water sources, by means of water recycling and re-use. Though the government is encouraging water recycling and re-use, it is not implemented effectively in India. At present, even for gardening, vehicle washing, fire protection etc., fresh/potable water is used. More than 70% of the water drawn from the source is used and let into sewer lines as waste water. If the same is properly treated and recycled then there will be little reduction in drawing the fresh water.

Water Pollution in India

General

Water pollution in India can be classified in different ways which is highlighted from the following section. First, bacterial pollution is widespread in India which produce fatal illness of death (through waterborne diseases) of almost 40 million peoples/year [22]. Second, more than 90% of the sewage generated by rural municipalities and more than 50% of sewage discharged by urban municipal go untreated and discharged to the fresh water ecosystem [27,32]. Third, industry produces pollutants that are extremely harmful to people, wildlife and the environment. Furthermore several of industrial facilities in India use freshwater to carry away waste from the plant and into rivers, lakes and oceans. Especially, industries produce nearly 31,000 million cubic meters of effluent which is discharged into our fresh water bodies [28]. Fourth, in India, the estimated fecal load is 200.000 tones are generated

severely affected. Arsenic (As) contamination was reported in ground water in several parts of the country in which West Bengal is heavily contaminated (60% of the districts are contaminated), affecting 26 million people [33]. The presence of arsenic, a poison and a carcinogen, in the groundwater of the Ganges delta causes health risks to 35–60 million people in West Bengal and Bihar. Researchers have found elevated levels of arsenic in the soil and groundwater near a gold mine in Karnataka (Kiradalli Tanda village of Yadgir district), India [34]. The research also highlights health hazards associated (arsenic induced skin disease and cancer) with mining because of arsenic contamination in groundwater found to 30 to 200 times higher than the limit of 10 parts per billion (ppb), prescribed by the WHO [23]. An elevated concentration of total chromium (Cr) and hexavalent chromium (Cr-IV) is observed in wells in the industrial area in Chennai, Tamil Nadu [35]. The concentration of Cr in these wells varies between 3 to 250 mg/l whereas the concentration of Cr-IV ranged from 2 to 210 mg/l which far exceed the concentration of 0.05 mg/l prescribed under the Indian standard specification for drinking water quality [26]. In areas where water has high load of minerals like fluoride, arsenic and chrom... alternative sources (canal water, rain water harvesting) would ha... be provided not only for drinking water but also in farming. Periodic examination of water quality, particularly for the detection of fluori... arsenic and chromium is necessary in newer alluvium and flood ... areas in different parts of India. Water supplied by urban municipal... and rural Panchayats should be free of biotic and abiotic toxi... including micro elements and minerals.

Kurunthachalam et al, Indian Waters: Past and Present, Hydrol Current Res 2013, S10 DOI: 10.4172/2157-7587.S10-001

DownToEarth | डाउन टू अर्थ

42 rivers have extremely high concentration of neurotoxic heavy metals

Ganga was found to be polluted with five heavy metals, namely chromium, copper, nickel, lead and iron

By Kiran Pandey, Rajit Sengupta, Isha Bajpai

Last Updated: Tuesday 05 June 2018

India's 42 rivers have at least two toxic heavy metals beyond the permissible limit, says a research conducted by Central Water Commission.

The study, which tested samples of river water collected from 16 river basins during three seasons—summer, winter and monsoon—found huge amount of lead in 69 rivers. The study also showed that most rivers (137) had iron beyond permissible limits.

https://www.downtoearth.org.in/news/water/huge-amounts-of-toxic-heavy-metals-swim-in-indian-rivers-60545

Tuesday, 10 November 2020

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HEALTH HAZARD

Just 60% Punjab groundwater fit for use

CAG says it's laden with toxic chemicals, heavy metals

According to sources in the Department of Water Resources, the 26-page report will be tabled in the upcoming Budget session of the Punjab Vidhan Sabha from Thursday.

The CAG report says 40 per cent of the groundwater in the state is contaminated with chemicals and heavy metals beyond permissible limits. While 10 per cent of it is unsafe even for irrigation purposes, 30 per cent is marginally to moderately saline/alkaline, but can't be used by humans.

Heavy metal contamination

Lead: Amritsar, Bathinda, Ferozepur, Gurdaspur, Muktsar

Cadmium: Fatehgarh Sahib, Ludhiana, Nawanshahr, Patiala

Chromium: Sangrur, SAS Nagar, Tarn Taran, Amritsar,

Barnala, Bathinda, Gurdaspur, Kapurthala, Mansa, Ropar.

https://www.tribuneindia.com/news/punjab/just-60-punjab-groundwater-fit-for-use-43185

Major Categories of Water Pollutants

- Infectious Agents
  - Bacteria, Viruses, Protozoa, Parasitic Worms
  - Source: Human and animal waste
- Oxygen-Demanding Waste
  - Organic debris & waste + aerobic bacteria
  - Source: Sewage, feedlots, paper-mills, food processing
- Inorganic Chemicals
  - Acids, Metals, Salts
  - Sources: Surface runoff, Industrial effluent, household cleansers
- Radioactive Materials
  - Iodine, radon, uranium, cesium, thorium
  - Source: Coal & Nuclear Power plants, mining, weapons production, natural
- Plant Nutrients
  - Nitrates, Phosphates,
  - Source: Sewage, manure, agricultural and landscaping runoff
- Organic Chemicals
  - Oil, Gasoline, Plastics, Pesticides, Solvents, detergents
  - Sources: Industrial effluent, Household cleansers, runoff from farms and yards
- Eroded Sediment
  - Soil, Silt
- Heat/Thermal Pollution
  - Source: Power plants, Industrial

More than 50% of the population has no access to safe drinking water and about 200,000 people die every year for lack of access to safe water:

NITI Ayog Report 2020

THE ECONOMIC TIMES | News

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ADVERTORIAL

Times Water Summit 2020: It's still not late in saving India from becoming a waterless country if we start acting on it now!

The Times Water Summit 2020, a Times of India initiative under the banner of '**Make India Water Positive**', is spearheading the need for stronger and unified water infrastructure by bringing key stakeholders of the ecosystem –

the people, the policymakers, the corporates, and the agricultural community - all under one roof.

Permissible limits for the Hazards in Environment

- Permissible limits standardized by organizations like WHO, JECFA, OHSA etc.

Toxic elements	Permissible limits (ppm)	Effect of toxic elements on human health
Arsenic	0.01	Arsenic toxicity causes different diseases. High concentration of Arsenic is carcinogenic.
Cadmium	0.003	High concentration of cadmium causes kidney and liver damage, anemia, carcinogenic, retard growth and also causes renal arterial hypertension.
Chromium	0.05	Chromium is carcinogenic, causes lung cancer and genotoxic in nature.
Lead	0.01	Affects peripheral nervous system and central nervous metabolism. High concentration of lead is carcinogenic.
Mercury	0.001	Inorganic Mercury compounds affect kidney and nervous system disorders, oral poisoning causes haemorrhagic gastritis and colitis. Carcinogenic on high concentration

– Singh et al 2018, Water purification by using Adsorbents: A Review S2352-1864 (17)30266-3

Permissible limits for the Hazards in Environment

TICs	PEL (ppm)	Extrapolated LOD (ppm)
Ammonia	50	0.08
Arsine	0.05	0.01
Chlorine	1	0.01
Diborane	0.1	0.01
Dimethylamine	10	0.01
Fluorine	0.1	0.01
Formaldehyde	0.75	0.12
Hydrogen chloride	5	0.02
Hydrogen cyanide	10	0.02
Hydrogen fluoride	3	0.02
Hydrogen sulfide	20	0.08
Hydrazine	1	0.01
Methylamine	10	0.01
Methyl hydrazine	0.2	0.01
Nitric acid	2	0.02
Nitrogen dioxide	5	0.03
Phosgene	0.1	0.01
Phosphine	0.3	0.01
Sulfur dioxide	5	0.06
Trimethylamine	10	0.03

Sensor

A sensor is a device that detects events or changes in quantities and provides a corresponding output, generally as an electrical or optical signal.

One might consider the ears, eyes, nose and fingers to be physical sensors as they detect physical sensations of sound, light, smell and heat respectively.

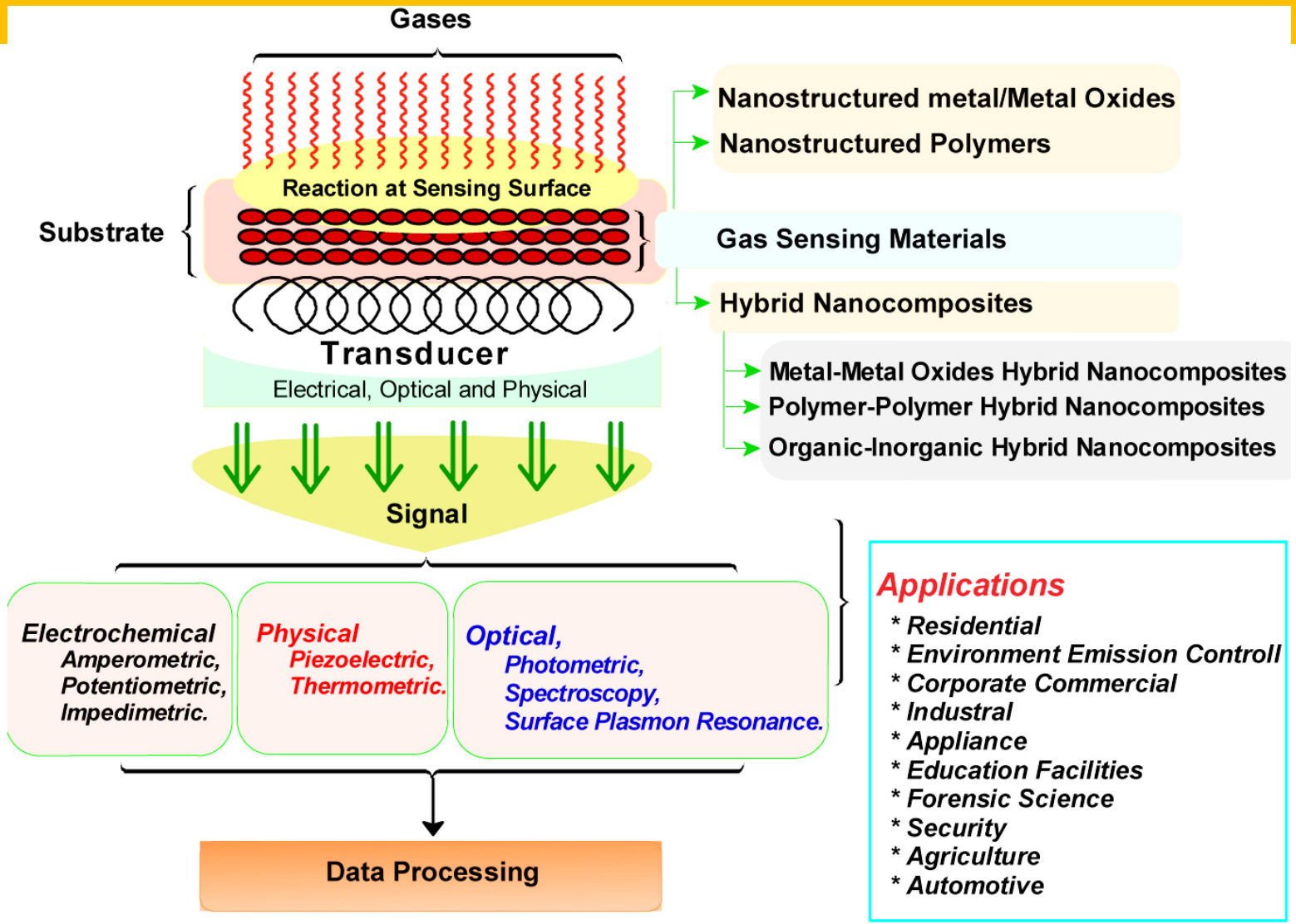
Understanding Sensor:

A device for sensing a physical variable of a physical system for an environment.

Mechanical parameter: Displacement, Strain, Rotation velocity, Acceleration, Pressure, Force/Torque, Twisting, Weight, Flow
Thermal parameter: Temperature, Heat.
Electromagnetic/optical parameter : Voltage, Current, Frequency phase, Visual/Images, Light, Magnetism.
Chemical parameter : Moisture, pH value

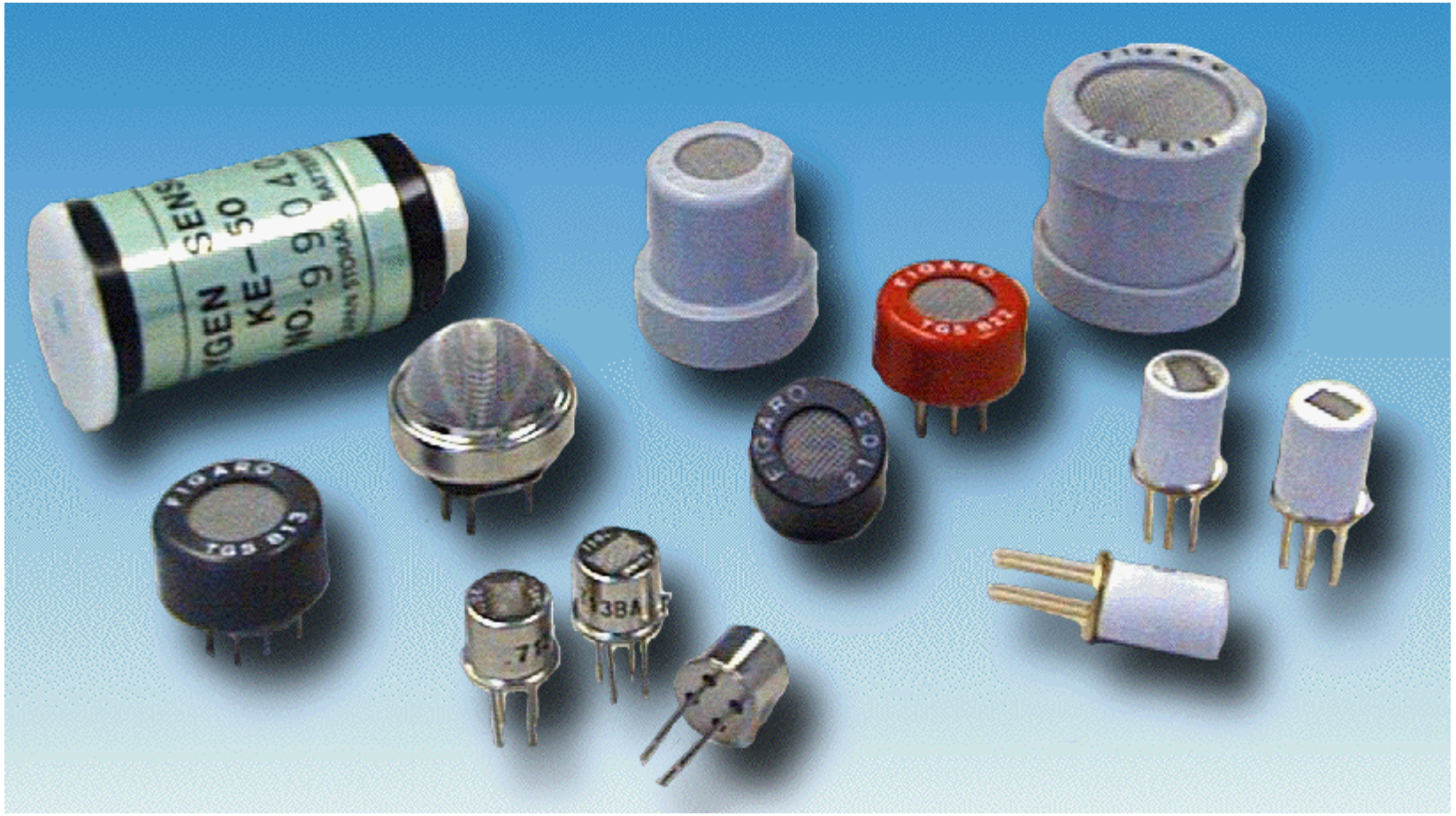
Sensors are required in many areas:

Environment Pollution: **Our Focus is On Toxic Gases**
Water Pollution: **Heavy metals in water**
Noise Pollution:
Automobile, Industry, Health, Robotics etc.
Biomarkers for Cancer and Diabetes



Kaushik A, Kumar R, Arya SK, Nair M, Malhotra B, Bhansali S. Organic-Inorganic Hybrid Nanocomposite-Based Gas Sensors for Environmental Monitoring. Chemical reviews 2015;115(11):4571-606.

Various gas sensors

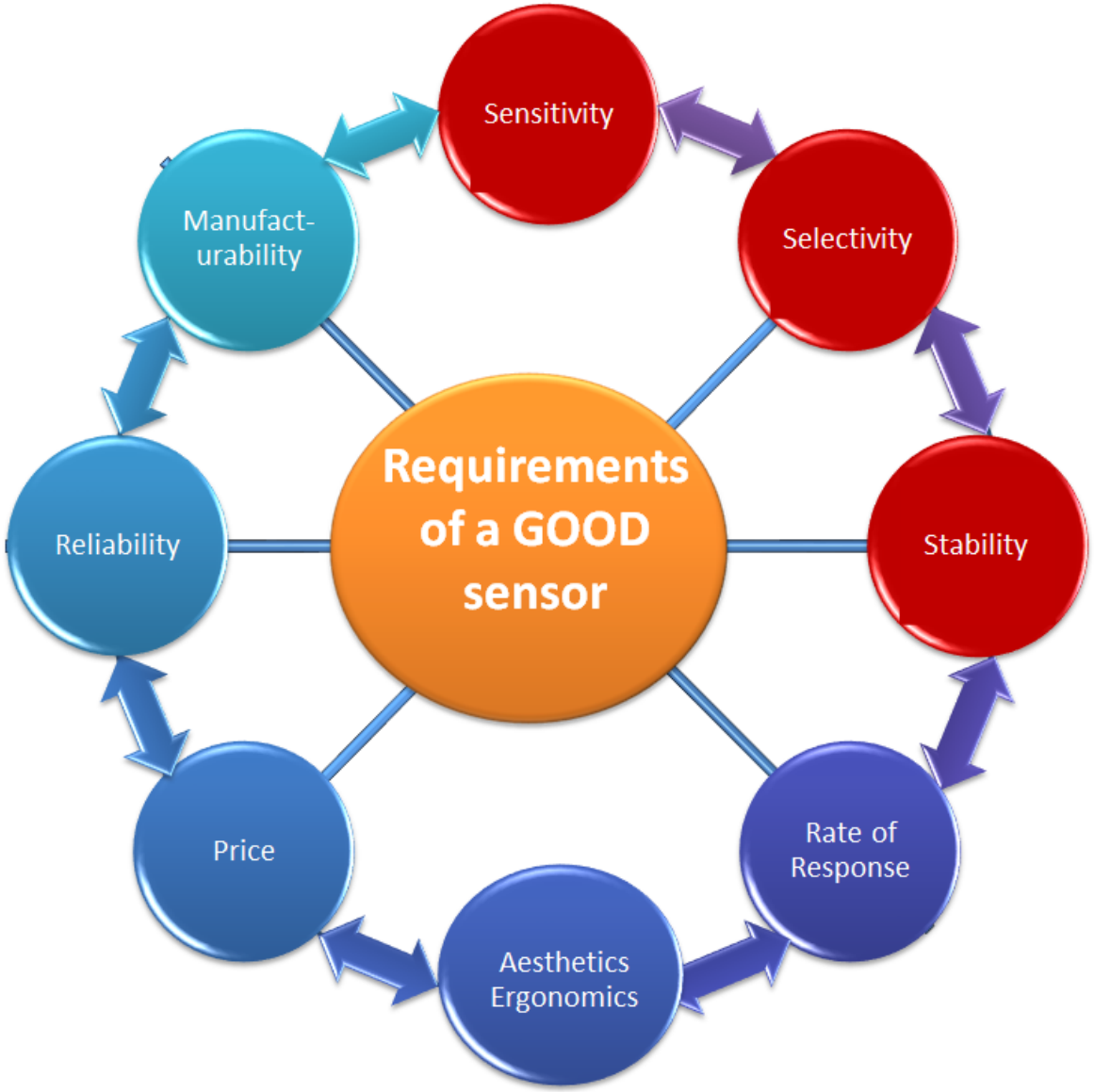


Primitive Concept

The canary, normally a very songful bird, is more susceptible than humans to low oxygen, methane gas, or CO gas. Because of its highly sensitive nature towards gases, people used them to detect poisonous gases in mines. They would stop singing and eventually die in the presence of these gases.

Application: Gas/Chemical sensor

- **Safety in Domestic, Industrial and Strategic sectors**
  - *Detection of flammable gases like LPG, CNG, methane, hydrogen*
  - *Detection of toxic gases like CO, NH_3, H_2S*
  - *Fire / Smoke detection*
  - *Explosive Detection*
  - *Nerve Gas / Poison Gas Detection*
- **Monitoring Environmental (Air/water) Pollution and Control**
  - *SO_x, NO_x, CO, HC, CO_2 etc.*
  - *Halocarbons like CFC*
  - *Heavy Metals (As, Cd, Zn, Pb etc.)*
- **Food and Agriculture**
  - *Food Quality Detection (Freshness of Fruits, Fishes etc.)*
  - *Odor Detection (Sulphides, Amines etc.)*
- **Advance biomedical application**
  - *Breath Alcohol Analyzers*
  - *Diabetes Sensors*



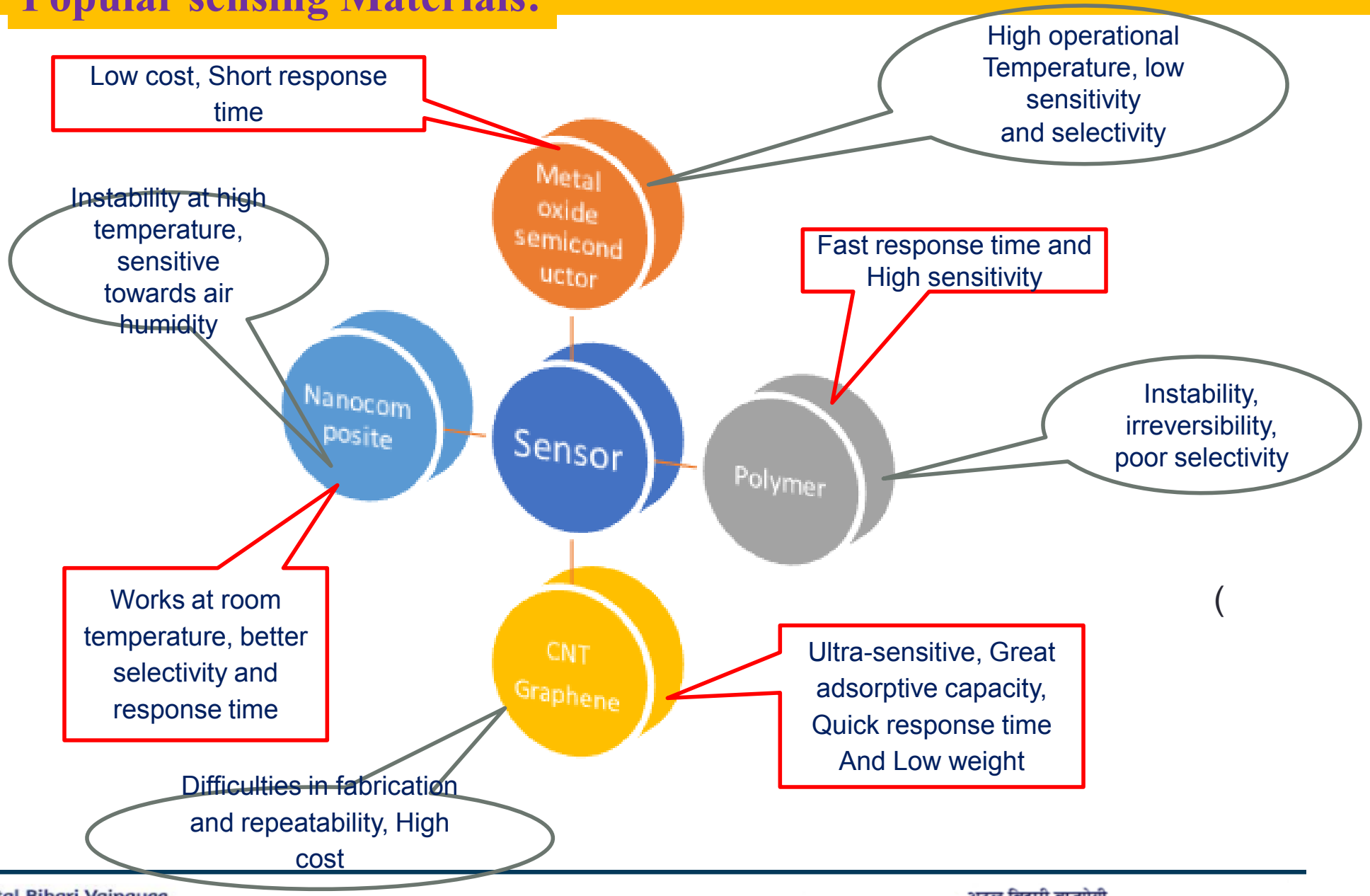
Sensitivity is a change of measured signal per analyte concentration unit, i.e., the slope of a calibration graph. This parameter is sometimes confused with the detection limit.

Selectivity refers to characteristics that determine whether a sensor can respond selectively to a group of analytes or even specifically to a single analyte.

Stability is the ability of a sensor to provide reproducible results for a certain period of time. This includes retaining the sensitivity, selectivity, response, and recovery time.

Response time is the time required for sensor to respond to a step concentration change from zero to a certain concentration value.

Popular sensing Materials:



Nanomaterials: Due its Size and Shape

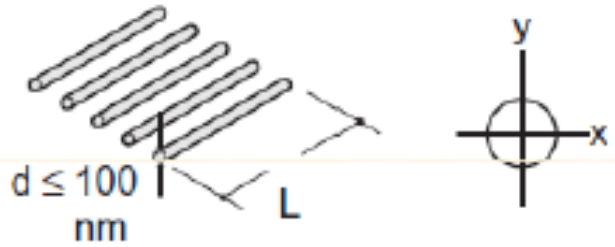
0-D

All dimensions (*x*,*y*,*z*) at nanoscale

Nanoparticles

1-D

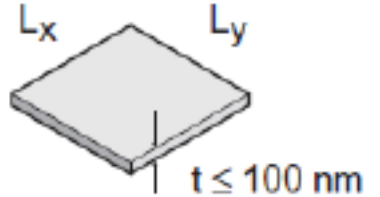
Two dimensions (*x*,*y*) at nanoscale, other dimension (*L*) is not



Nanowires, nanorods, and nanotubes

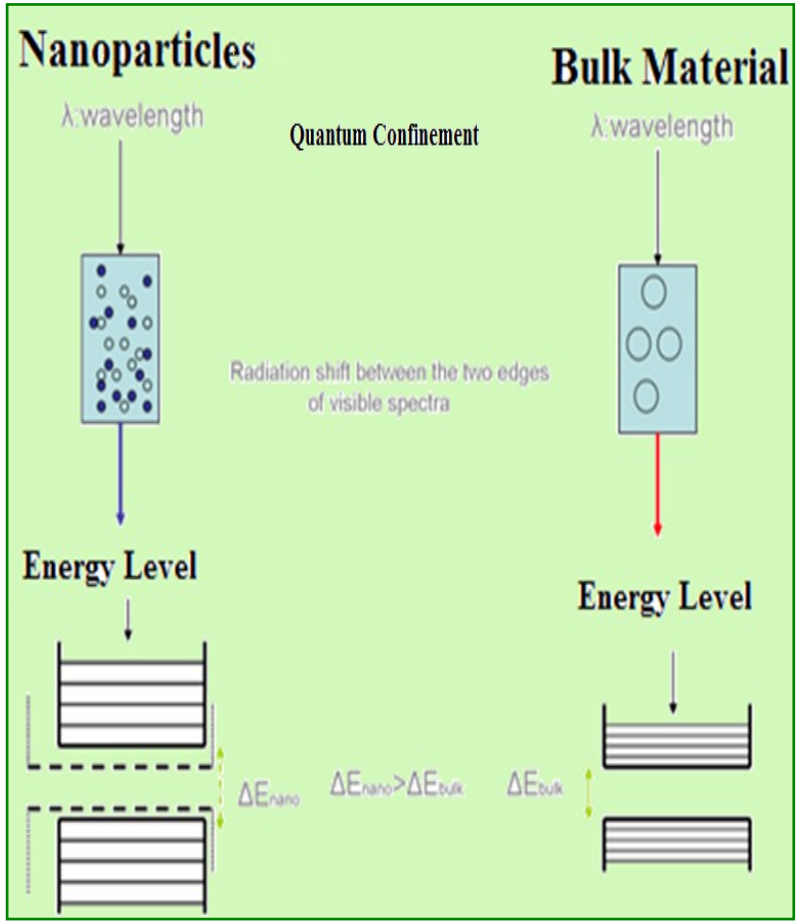
2-D

One dimension (t) at nanoscale, other two dimensions- (L_x, L_y) are not

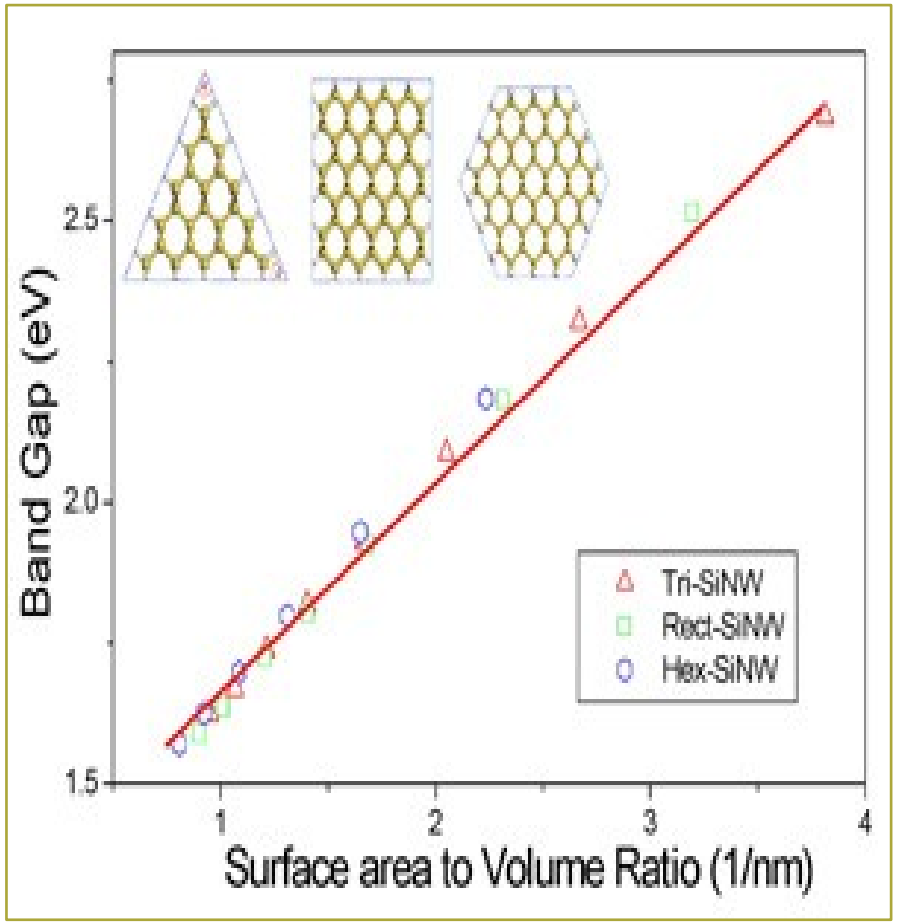


Nanocoatings and nanofilms

Two Reasons makes difference:

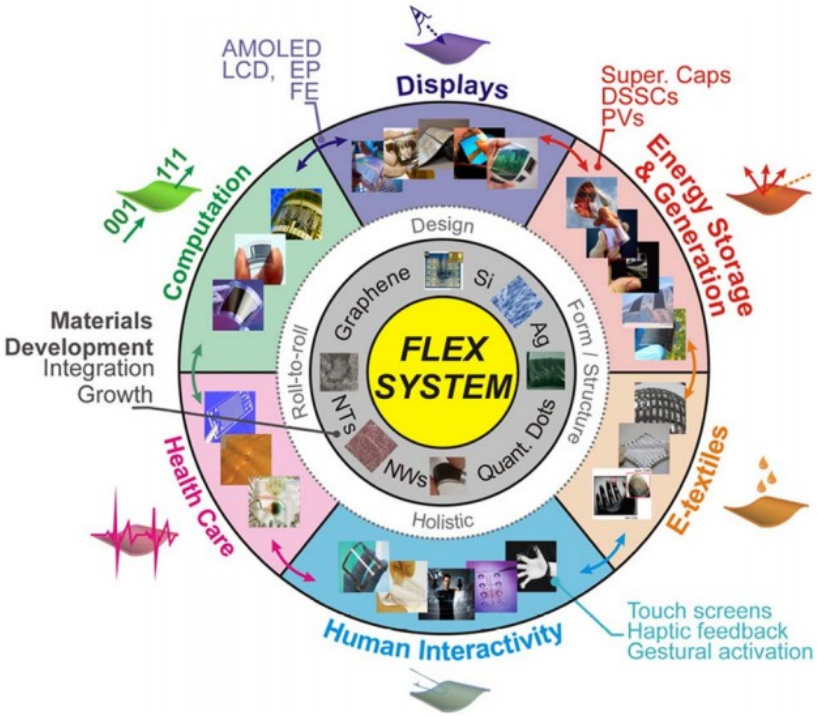


Quantum Confinement

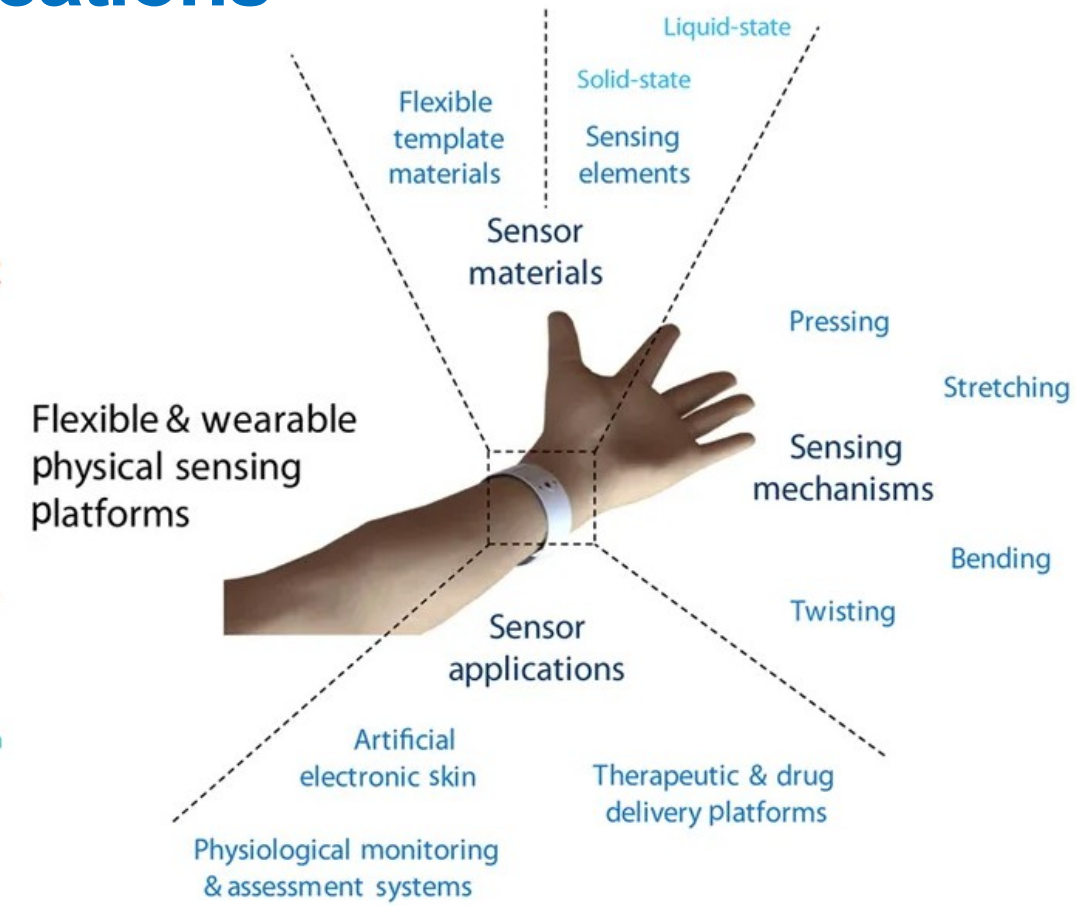


Surface to volume ratio

Nanomaterials: Applications



Arokia Nathan, Arman Ahnood, Matthew T. Cole, et al., Proceedings of the IEEE, **Vol. 100**, (2012)



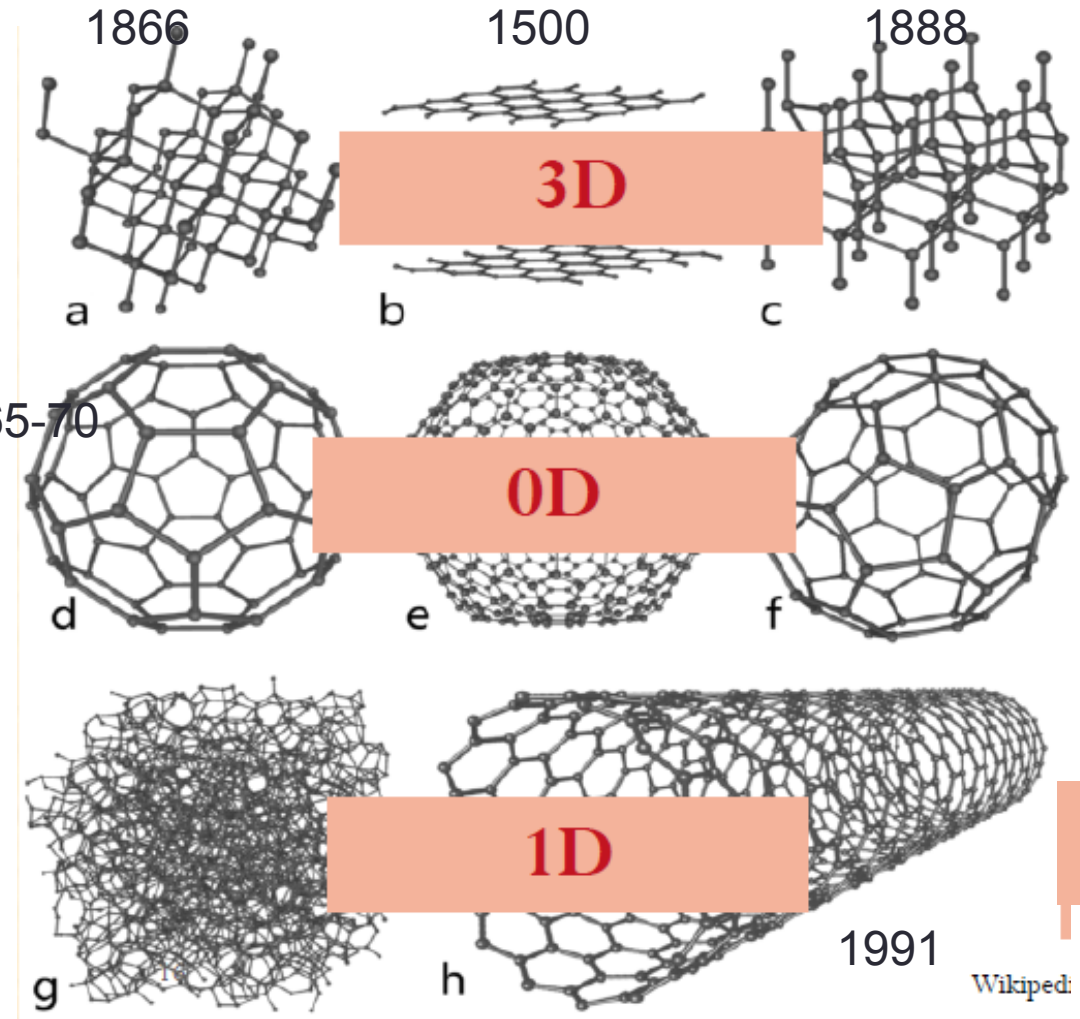
[Kenry](), [Joo Chuan Yeo]() & [Chwee Teck Lim](), *Microsystems & Nanoengineering* **Vol 2**, Article number: 16043 (2016).

Carbon: a material of interest

- Carbon is a basic element of life
- Carbon is special because of its ability to bond to many elements in many different ways
- It is the sixth most abundant element in the universe
- The most known types of carbon materials:
  - diamond;
  - graphite;
  - fullerenes; and
  - Carbon nanotubes

Most known Carbon:

From Early 1500 to1866 - 2010

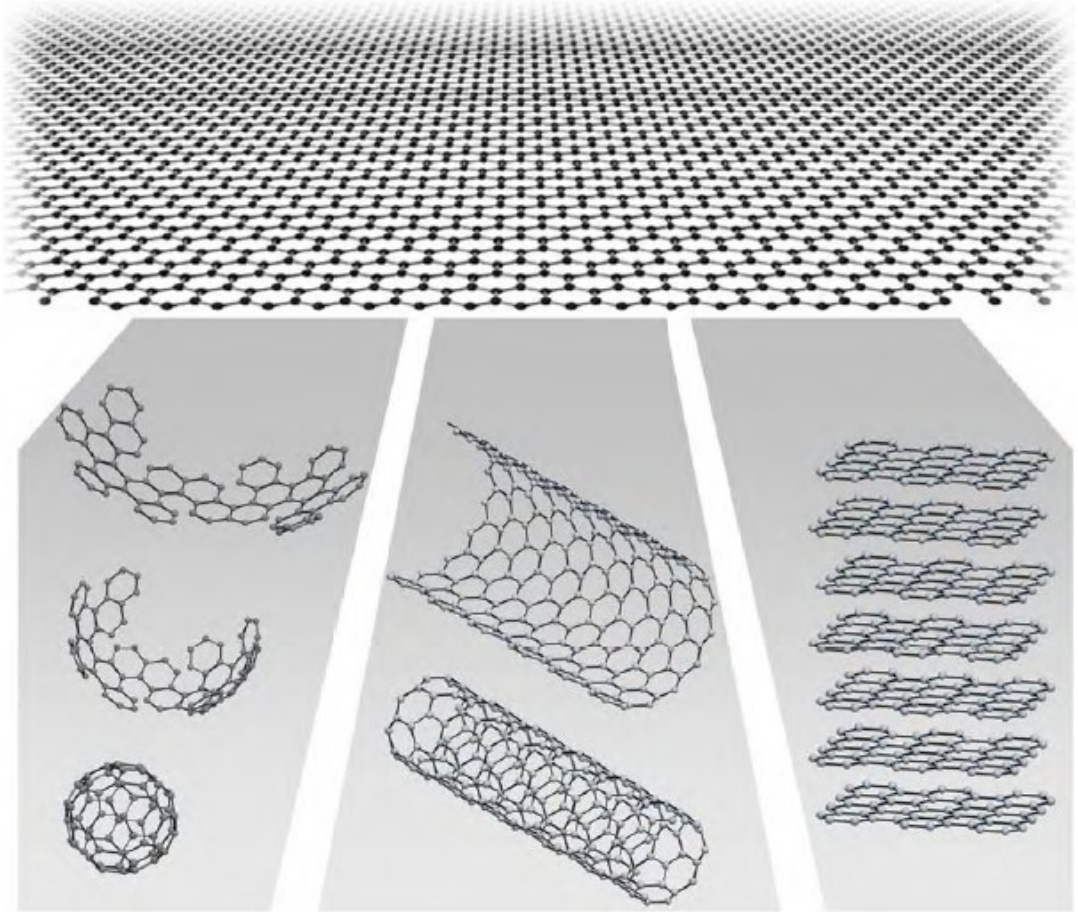


a) diamond
b) graphite
c) lonsdaleite (hexagonal diamond)
d) - f) fullerenes (C60, C540, C70);
g) amorphous carbon
h) carbon nanotube

2D - ???

2004, Prof. Andre Geim and Prof. Konstantin Novoselov

Graphene: The mother of all Graphites



Graphene is a 2D building material for carbon materials of all other dimensionalities. It can be wrapped up into 0D buckyballs, rolled into 1D nanotubes or stacked into 3D graphite.

2D-Nanostructure

Grpahene Sheet (0-Gap semiconductor)
Boron Nitride Sheet (~4.8eV)

} Flattened

Silicene
Germenene
Phospherene

} Buckled/ Puckered

1)Black Phospherene : single layer (Direct Band-Gap) (~1.88eV)

On increasing layers it goes upto 0.3eV (2014)

2)Blue Phospherene (Indirect Band-Gap) (~2eV) 2015

(displacement of some atoms from crystal phospherene → blue phospherene)

Arsenene (Theoretically simulated but experimentally not verified)
Antimonene (Theoretically simulated but experimentally not verified)
Borophene (Theoretically simulated but experimentally not verified)

} Buckled

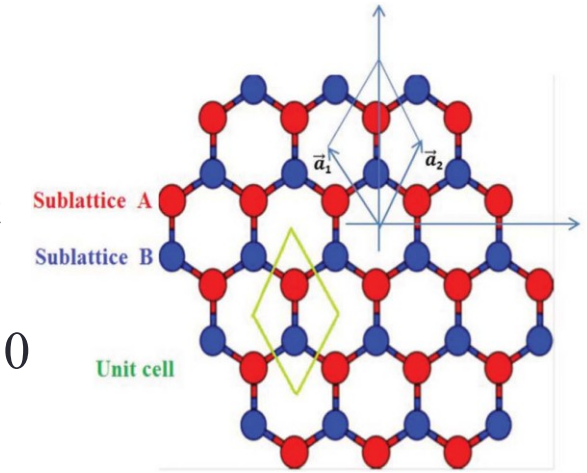
Graphene

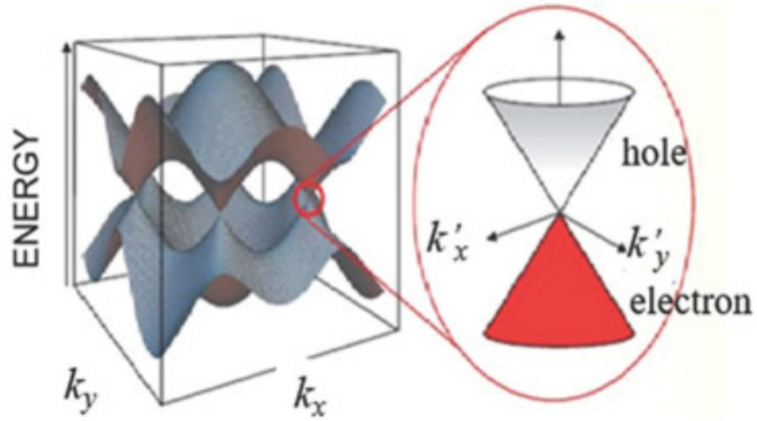
- Two carbon atom are present per unit cell
- Large surface area reported upto 2,630 m^2g^{-1}
- High carrier mobility is measured to be

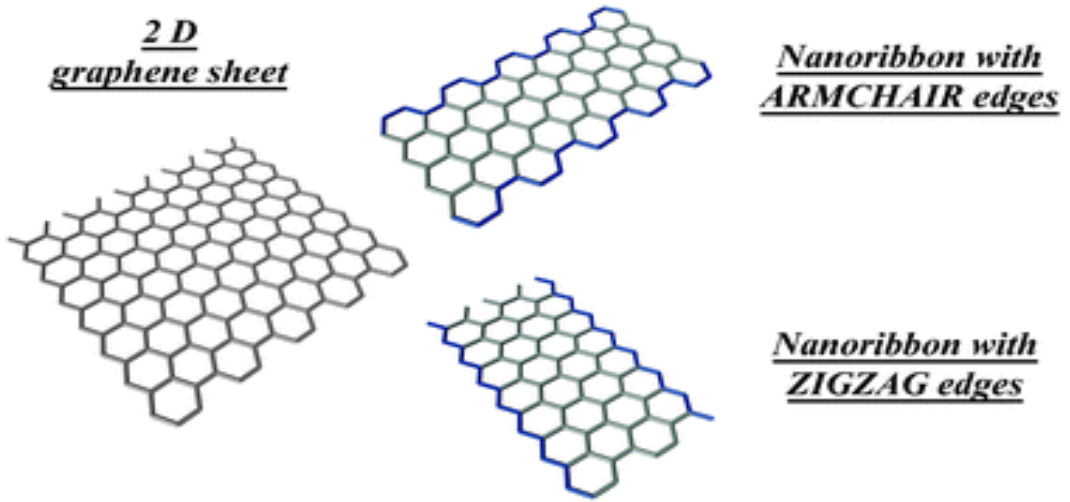
  experimentally ~15,000 $cm^2V^{-1}s^{-1}$ and

  theoretically ~2,00,000 $cm^2V^{-1}s^{-1}$
- Zero gap semiconductor in which valance band

  and conduction band meets at Dirac point.







K. S. Novoselov, A. K. Geim, N. M. R. Peres, F. Guinea and A. H. Castro Neto Reviews of Modern Phy, Vol 81, (2009).

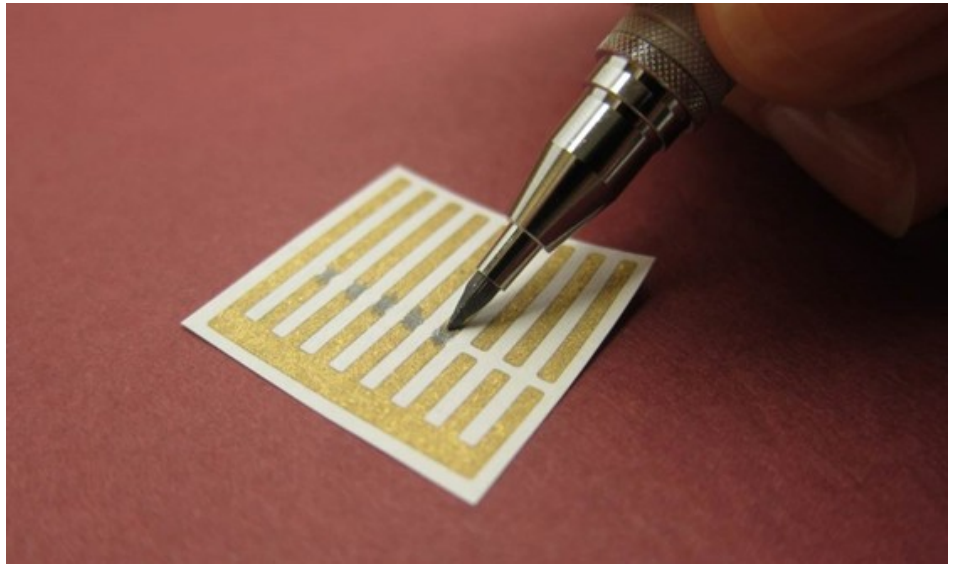
CNT as Sensor in 2013

- Carbon nanotubes offer a powerful new way to detect harmful gases in the environment.

But Challenge!!!!

Methods typically used to build carbon nanotube sensors are challenging.

MIT's Carbon Nanotube Pencil Draws Delicate Sensors onto Paper (2013)



Graphene as Sensor in 2007

nature materials

Letter abstract

Nature Materials **6**, 652 - 655 (2007)
Published online: 29 July 2007 | doi:10.1038/nmat1967

Subject Categories: Electronic materials | Sensors and biosensors | Nanoscale materials

Detection of individual gas molecules adsorbed on graphene

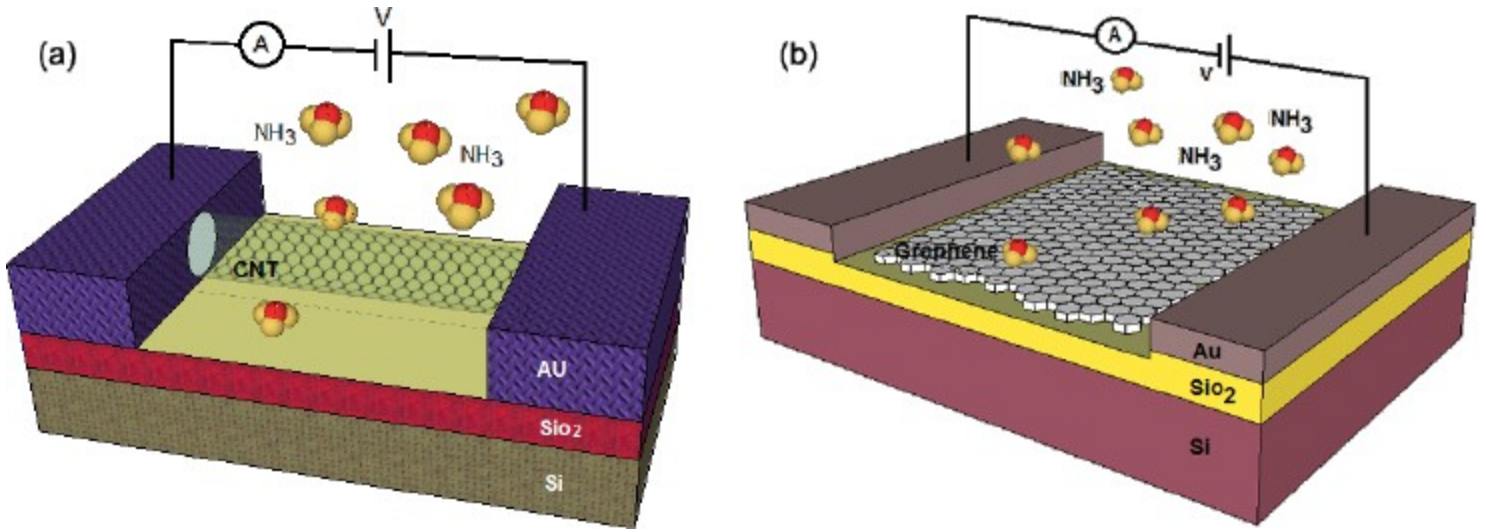
F. Schedin[1], A. K. Geim[1], S. V. Morozov[2], E. W. Hill[1], P. Blake[1], M. I. Katsnelson[3] & K. S. Novoselov[1]

The ultimate aim of any detection method is to achieve such a level of sensitivity that individual quanta of a measured entity can be resolved. In the case of chemical sensors, the quantum is one atom or molecule. Such resolution has so far been beyond the reach of any detection technique, including solid-state gas sensors hailed for their exceptional sensitivity[1, 2, 3, 4]. The fundamental reason limiting the resolution of such sensors is fluctuations due to thermal motion of charges and defects[5], which lead to intrinsic noise exceeding the

top

- **The density functional theory** (DFT) is presently the most successfull (and also the most promising) approach to compute **the electronic structure of matter**.
- Its **applicability** ranges from **atoms, molecules and solids** to **nuclei and quantum and classical fluids**.
- In its original formulation, the density functional theory provides **the ground state properties of a system**, and the **electron density** plays a key role.
- **An example: chemistry**. DFT predicts a great variety of molecular properties: molecular structures, vibrational frequencies, atomization energies, ionization energies, electric and magnetic properties, reaction paths, etc.
- **The original density functional theoy has been generalized** to deal with many different situations: spin polarized systems, multicomponent systems such as nuclei and electron hole droplets, free energy at finite temperatures, superconductors with electronic pairing mechanisms, relativistic electrons, time-dependent phenomena and excited states, bosons, molecular dynamics, etc.

Material Modeling for Air and water Pollution @ AMRG, IIITM Gwalior


(a)
A
V
NH3
NH3
CNT
AU
Sio2
Si
(b)
A
V
NH3
NH3
NH3
Graphene
Au
Sio2
Si

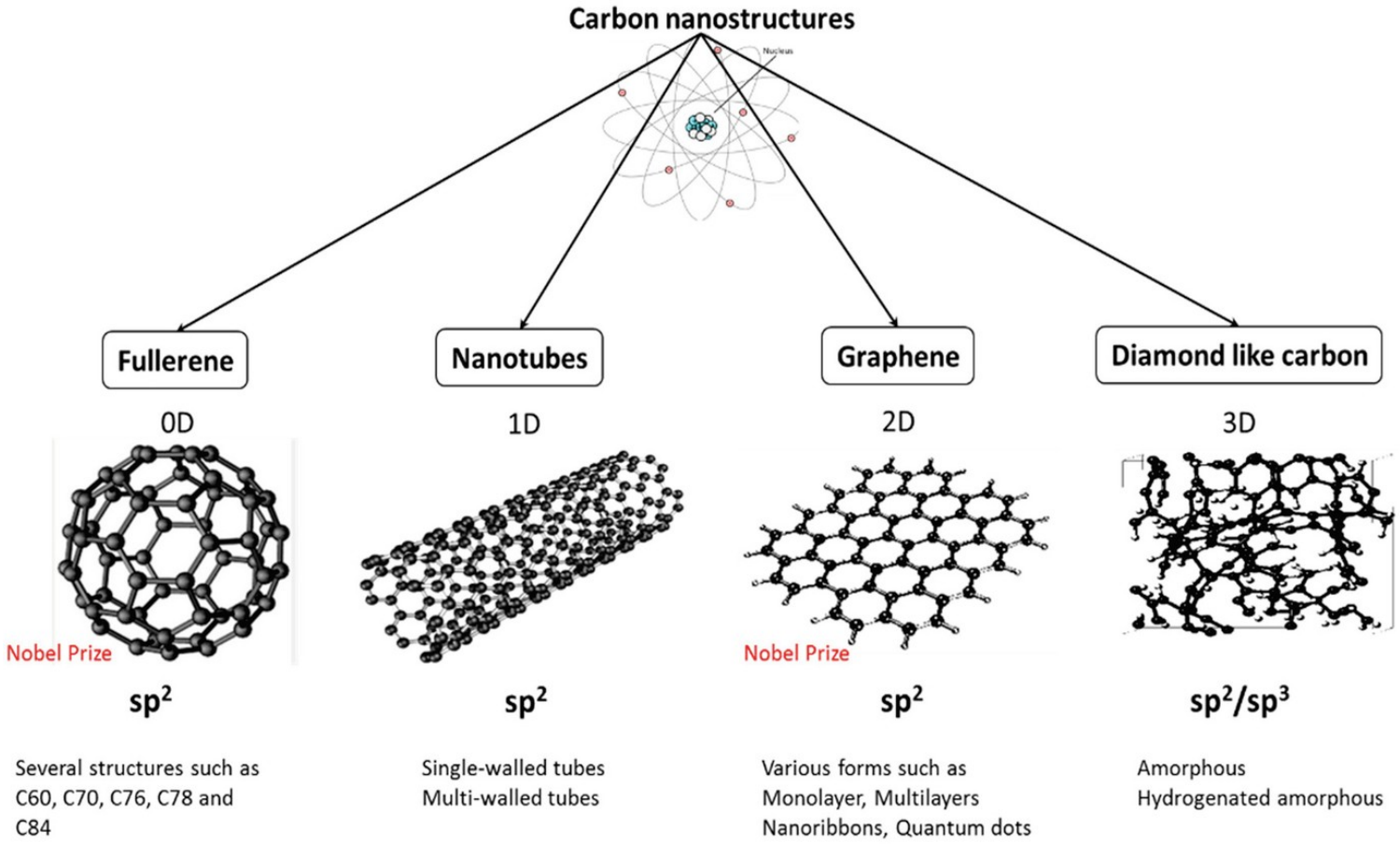
Research Gaps

Sensor related Challenges

- **Low conductivity** and **stability** of most common and studied metal oxide and polymer based sensors.
- Issues on **Sensitivity** to the extremely low concentration of gases/pollutants in environment→ early detection is not possible
- **Operational temperature** of the existing sensing devices very high
- **Selectivity** and **Recovery time** are other important challenges in existing sensors.
- Recent **efforts on using carbon materials are not enough** and have their own challenges in manufacturability etc.

TARGETED ADSORBENTS

Carbon Nanostructures



Sensor Modelling through *ab-initio* Approach.

1. Structural Stability
2. Adsorption Energy
3. Band structure and Density of State Analysis
4. Charge Transfer Analysis (Mullikan and NBO)
5. Conductance Analysis
6. Current Voltage Analysis
7. Sensitivity and response time

Air and water Pollution : Few 1D and 2D materials Analysis

METHODOLOGY

Considered Parameters to test the performance of modeled Sensor

- Adsorption energy (Stability, Endo/Exothermic nature)

$$E_{Ad} = E_{T(surface+molecule)} - E_{T(surface)} - E_{T(molecule)}$$

- Adsorption Mechanism (Physisorption / Chemisorption)
- Charge transfer (through Mulliken Population)

$$Q(e) = Q(surface + molecule) - Q(surface)$$

- Variation in electronic Properties (Band structure and DOS)
- Inter Frontial Orbital analysis (through HOMO-LUMO profiles)
- Conductance Analysis (Range of detection) $G = \int dE\, T(E) \frac{e^{(E-E_F)/k_BT}}{(1+e^{(E-E_F)/k_BT})^2}$
- Current-Voltage characteristics $I = \frac{2e}{h} \int_{\mu_L}^{\mu_R} [T(E)\{f_L(E) - f_R(E)\}] dE$

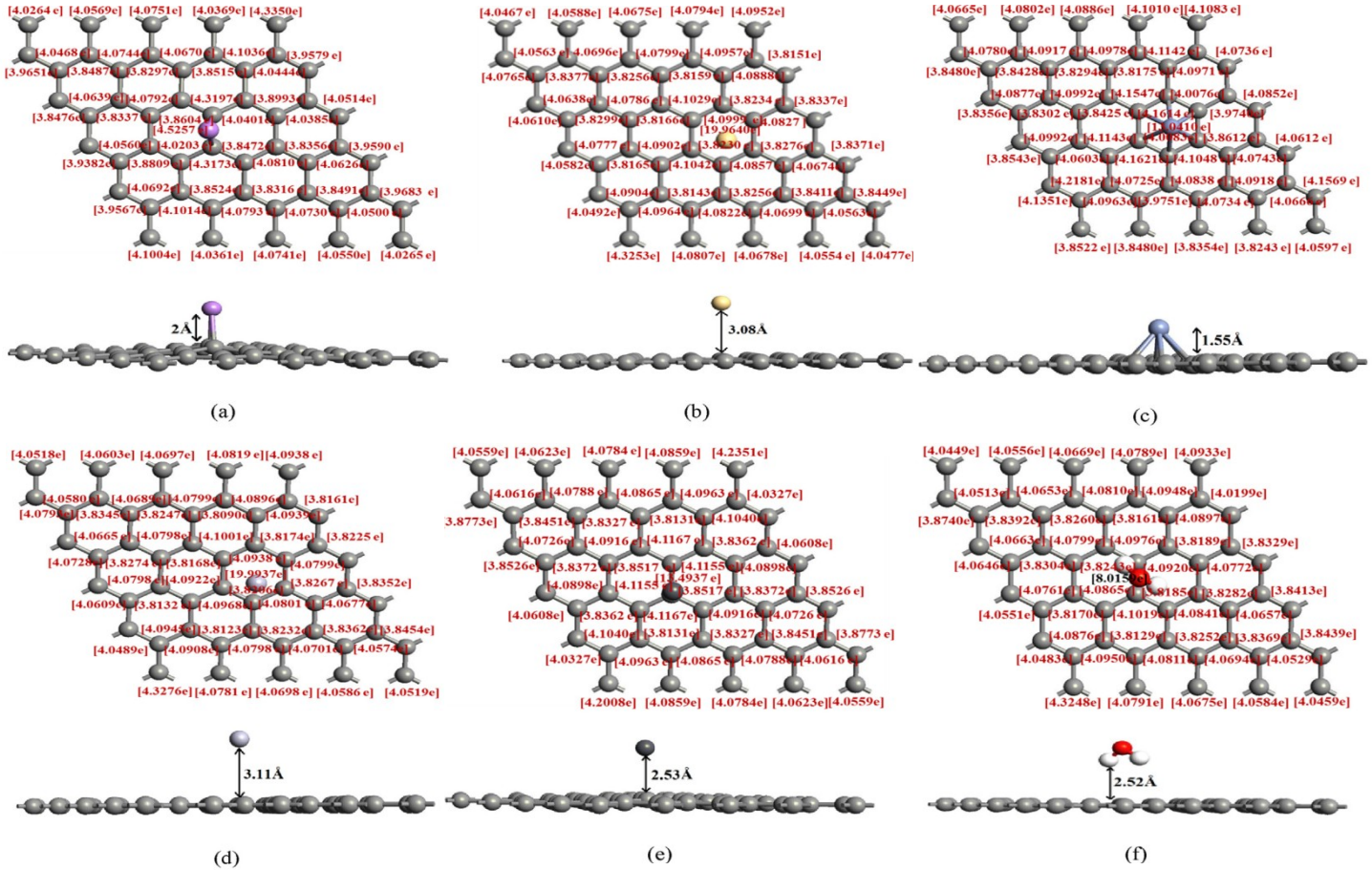
Recent Research on Detection of Water And Air Pollution Using Various Nanostructures

- Graphene and its derivatives are used for the detection of **carcinogenic heavy metals** (Arsenic, Cadmium, Chromium, Mercury, and Lead in water.
- Graphene and its derivatives are used for the detection **green house gases** CO_2, **toxic gases** like NH_3, Hydrogen halides, H_2S, etc.
- CNTs and its derivatives for the detection of **toxic gases** NH_3, Hydrogen halides (HF, HBr, HCl), H_2S, etc.
- Different Co-Polymers have been explored for **sensing cancer drugs**.
- Graphene and its derivatives are employed as a biosensors, like for the **detection of diabetes, breast cancer**.
- Defected Graphenes as **an supercapacitor, Single elearon devices**,
- **Spintronic** areas have also been explored.
- Different 1D materials for their application as **Interconnects**.

Suitability of Graphene Monolayer as Sensor for Carcinogenic Heavy Metals in Water: A DFT Investigation

Findings related to Detection of Heavy metals

Optimized Configuration of Heavy metal-Graphene complexes in Vacuum



Optimized structures of (a) As, (b) Cd, (c) Cr, (d) Hg, (e) Pb and (f) H_2O, adsorbed graphene in Vacuum.

M. Srivastava et al, Appl. Surf. Sci. 517 (2020) 146021. doi:10.1016/j.apsusc.2020.146021

Energetics of Heavy metal-Graphene complexes in Vacuum

Table 1
Adsorption energy (E_{ads}), Binding distance** of heavy metal from graphene sheet (d), and Charge transfer (Q_T).

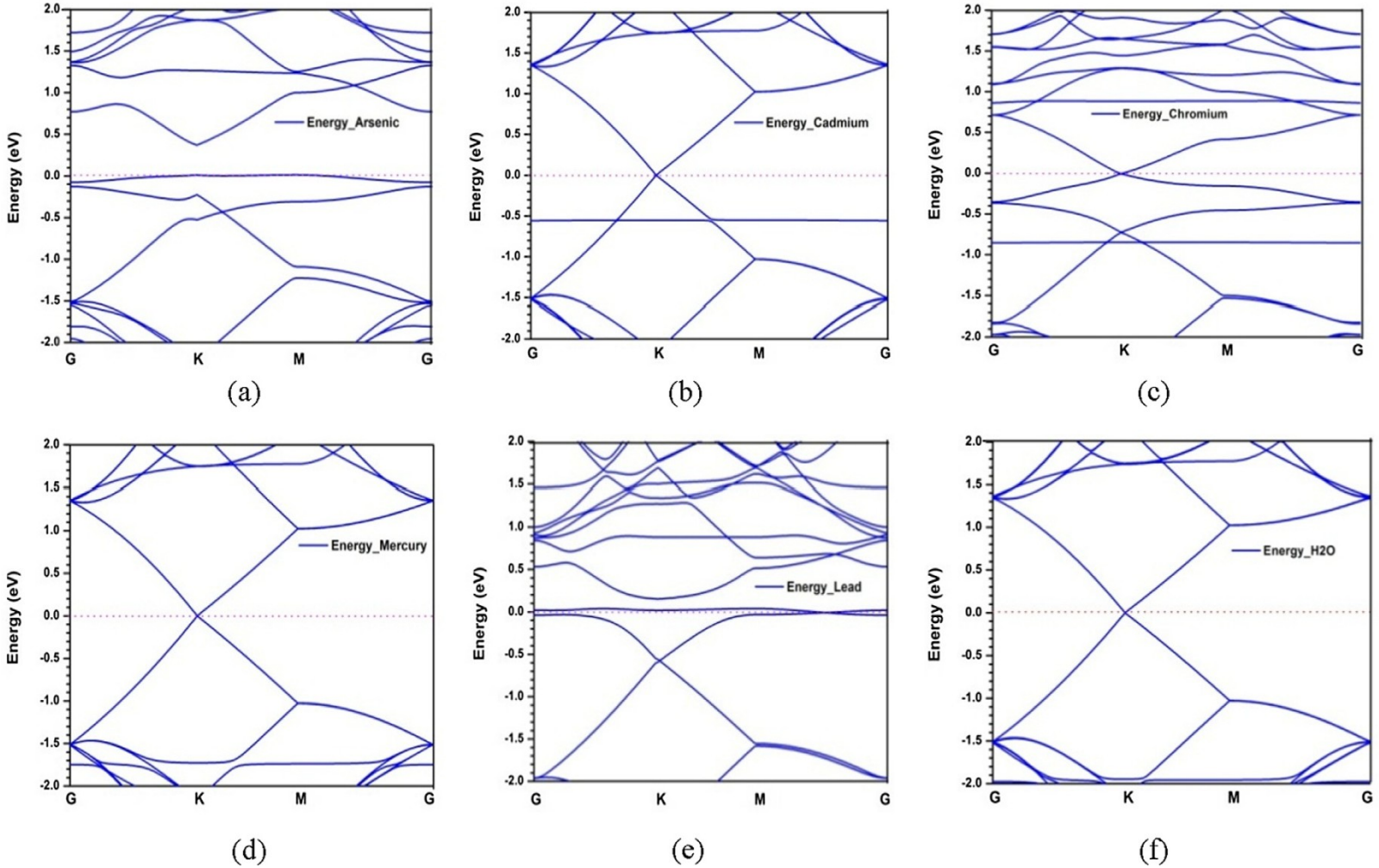
In Vacuum				In Water Environment		
Adsorbate	E_{ads} (eV)	d(Å)**	Bader Charge Q_{BT} (e)	E_{ads} (eV)	d(Å)**	Bader Charge Q_{BT} (e)
As	−1.39	2	−0.47	−0.97	2.08	−0.44
Cd	−0.23	3.08	−0.04	−0.31	3.14	−0.09
Cr	−2.55	1.55	−0.96	−2.14	1.54	−0.99
Hg	−0.26	3.11	−0.006	−0.32	3.17	−0.006
Pb	−0.91	2.53	−0.51	−0.97	2.18	−0.62
H_2O	−0.21	2.52	0.02*	–	–	

* Positive charge transfer means charge transfer took place from an adsorbent to adsorbate.

** Binding distance is defined as the minimum distance between the sheet and the adsorbate.

M. Srivastava et al, Appl. Surf. Sci. 517 (2020) 146021. doi:10.1016/j.apsusc.2020.146021

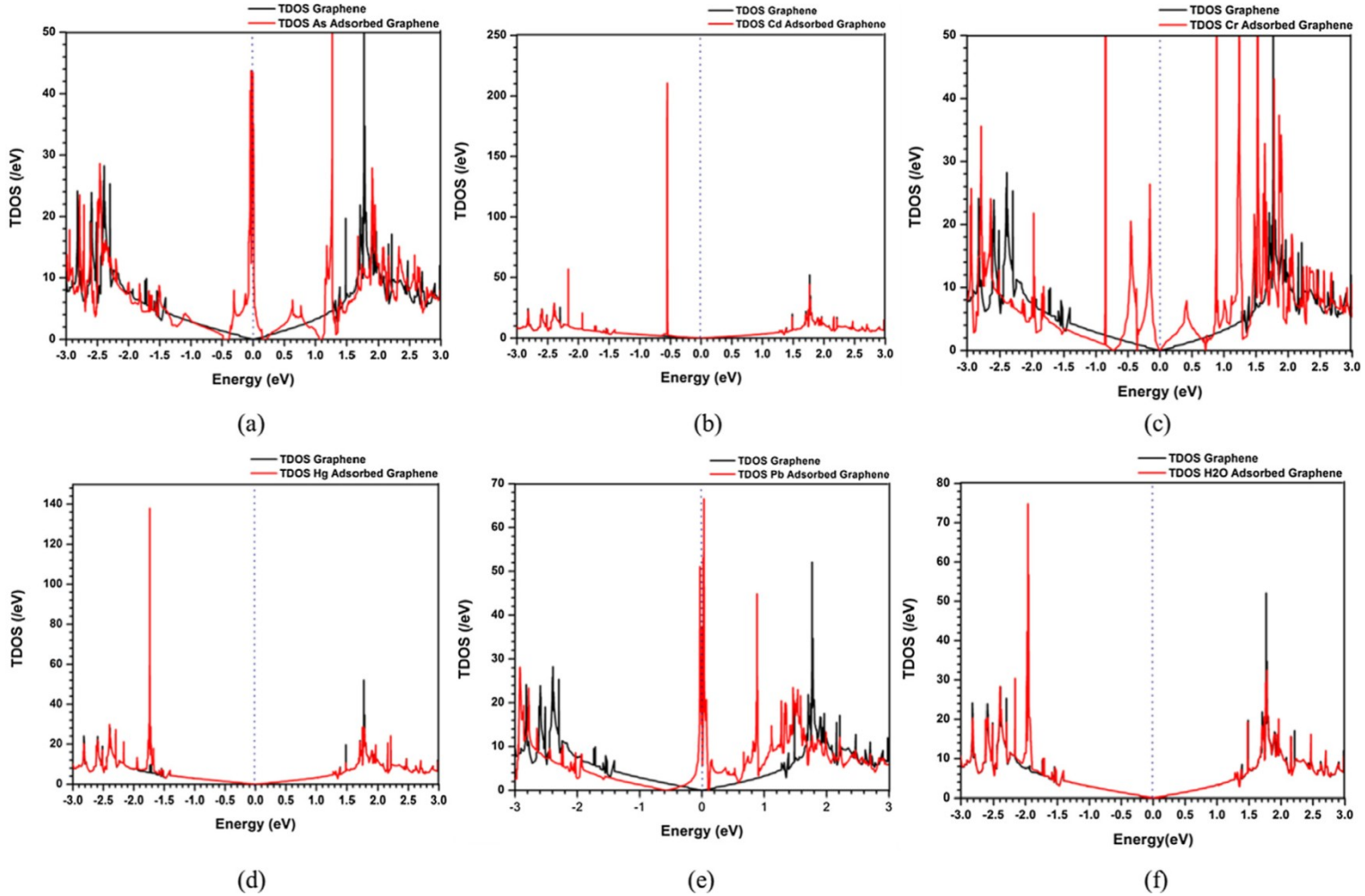
Electronic Band Structure Analysis



Band structure of graphene after adsorption of (a) As, (b) Cd, (c) Cr, (d) Hg, (e) Pb in Vacuum

M. Srivastava et al, Appl. Surf. Sci. 517 (2020) 146021. doi:10.1016/j.apsusc.2020.146021

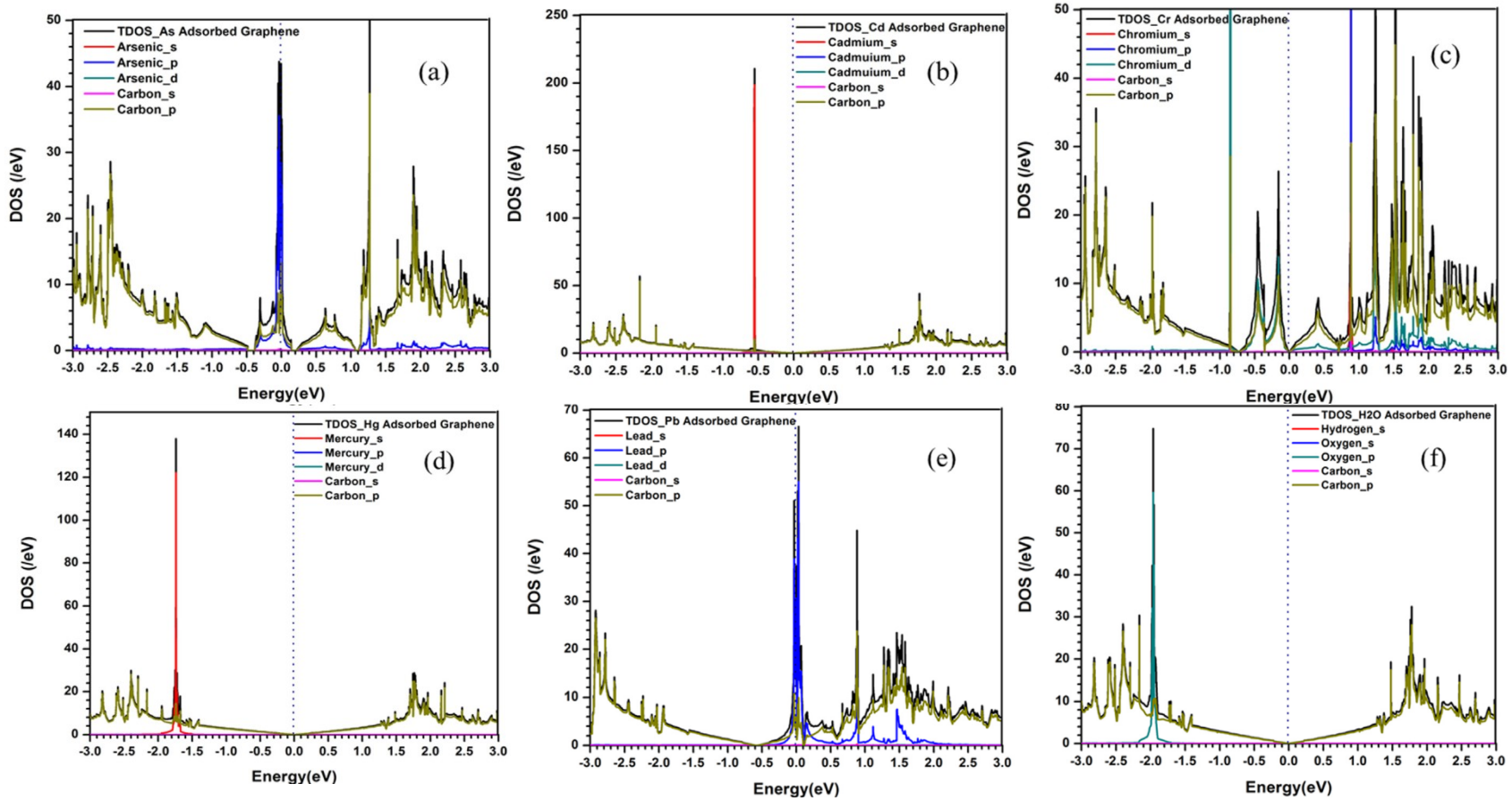
Comparison of Density of states Before and after adsorption of Heavy metal



Comparison of Density of states of graphene before and after adsorption of (a) As, (b) Cd, (c) Cr, (d) Hg, (e) Pb and (f) H_2O

M. Srivastava et al, Appl. Surf. Sci. 517 (2020) 146021. doi:10.1016/j.apsusc.2020.146021

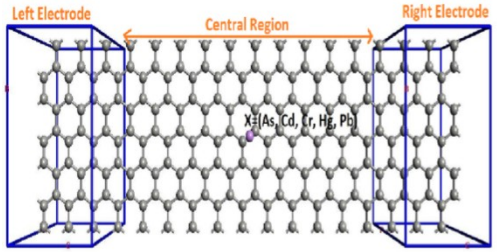
Partial Density of states profiles



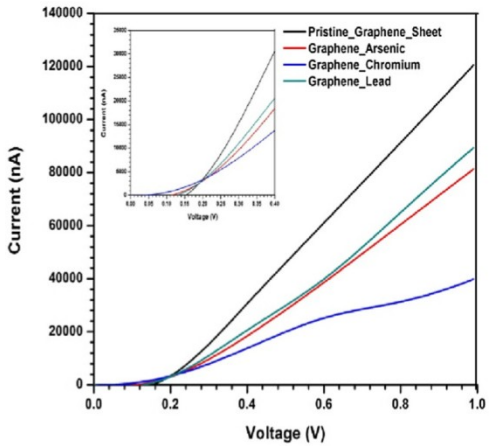
PDOS of Graphene sheet after adsorption of Heavy metals (a) As, (b) Cd, (c) Cr, (d) Hg, (e) Pb, and (f) H_2O.

M. Srivastava et al, Appl. Surf. Sci. 517 (2020) 146021. doi:10.1016/j.apsusc.2020.146021

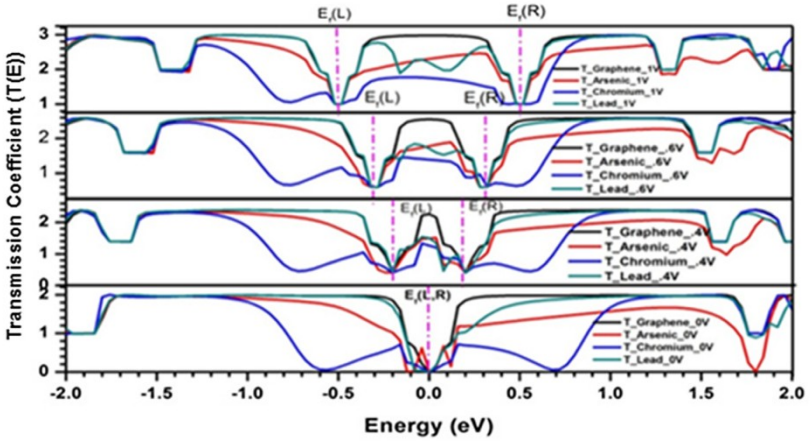
Electron Transport in Vacuum Environment



(a)

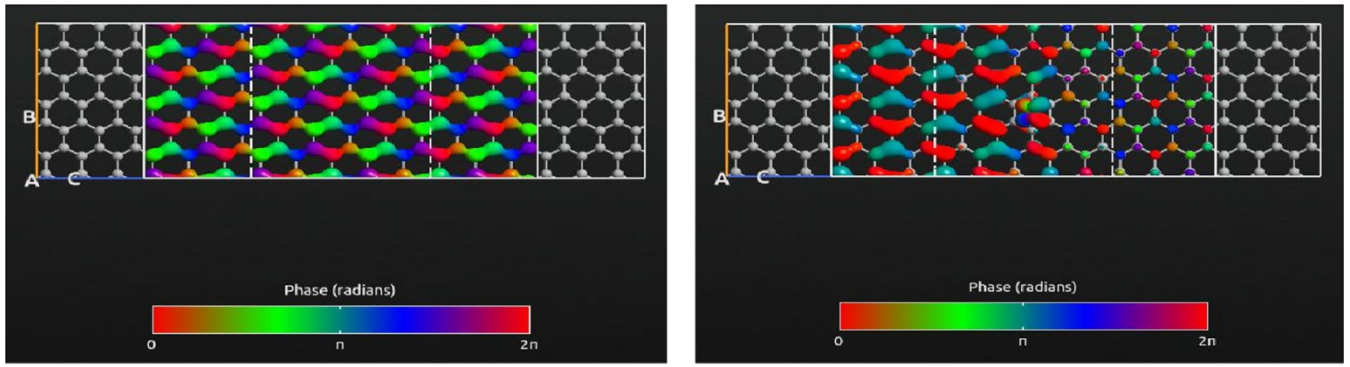


(b)



(c)

Schematic of two probe model of graphene based sensor system with isolated atom X (where X = As, Cd, Cr, Hg, Pb), (b) I-V Characteristics, (c) Transmission Spectrum of graphene sheet before and after adsorption of X = As, Pb



(a) (b)

Isosurface plots of the transmission eigenstates of (a) graphene and (b) Cr adsorbed graphene.

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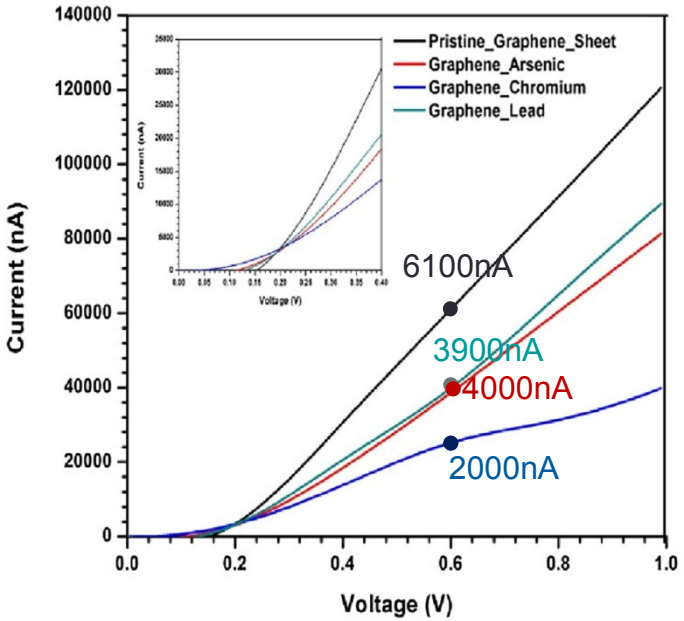
Sensing Parameter

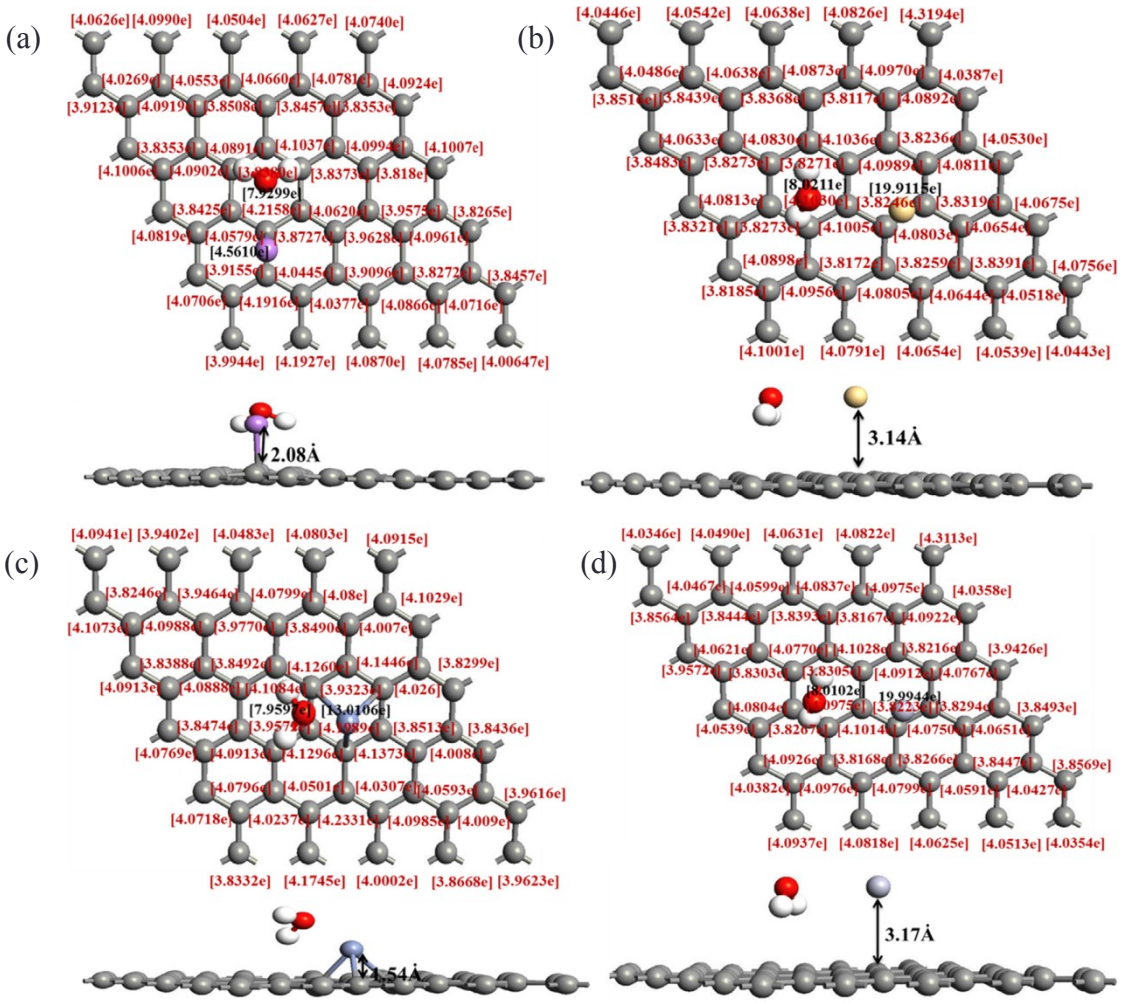


$$R(\%) = \frac{I_{Heavy\ metal} - I_{Graphene}}{I_{Graphene}} \text{x } 100$$

System	Response (%) (600mV)
Arsenic	36
Lead	59
Chromium	34

M. Srivastava et al, Appl. Surf. Sci. 517 (2020) 146021. doi:10.1016/j.apsusc.2020.146021

Optimized Configuration of Heavy metal-Graphene complexes in Aqueous Environment



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Optimized structures of (a) As, (b) Cd, (c) Cr, (d) Hg, (e) Pb, adsorbed graphene in Water environment.

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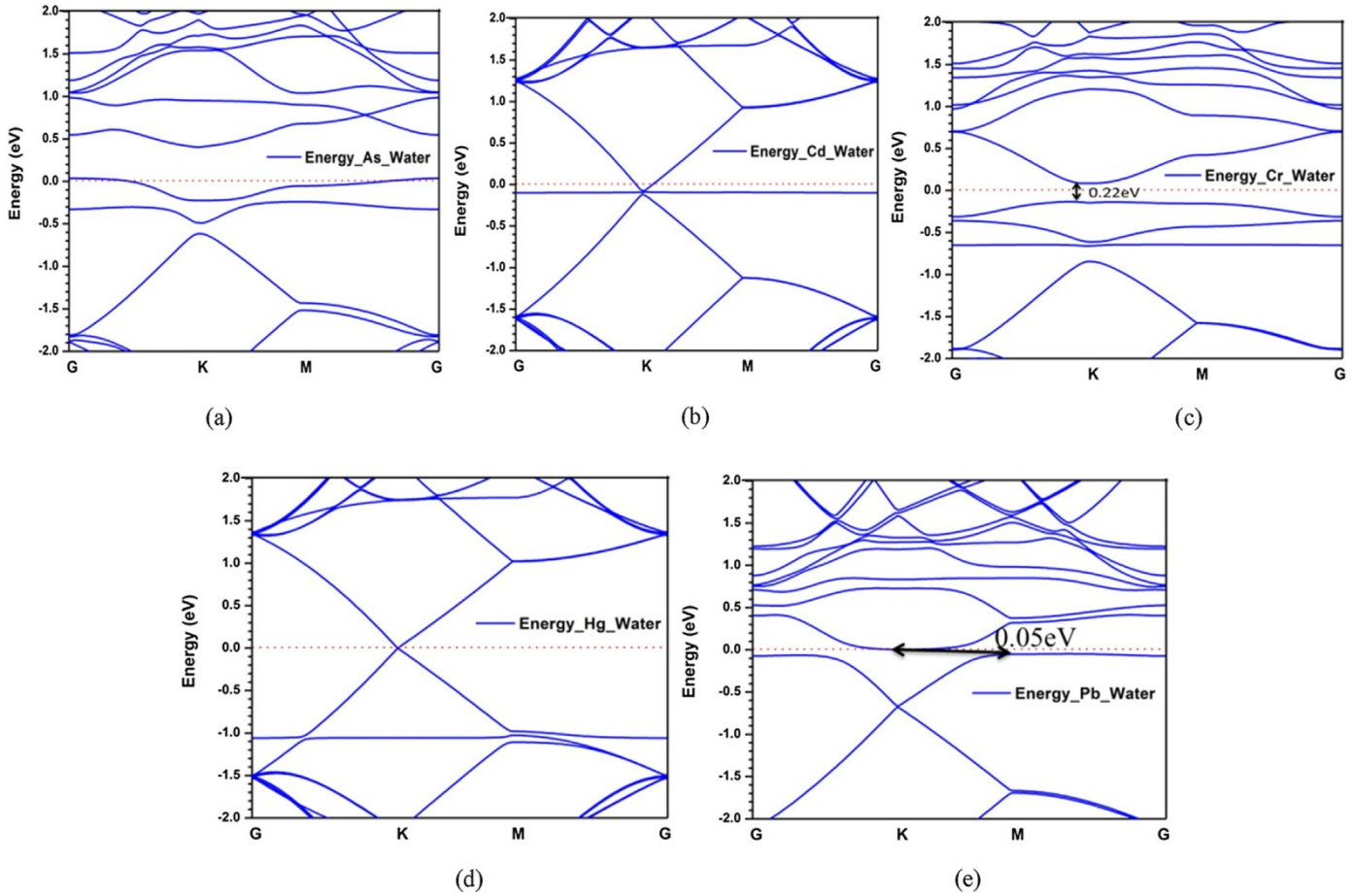
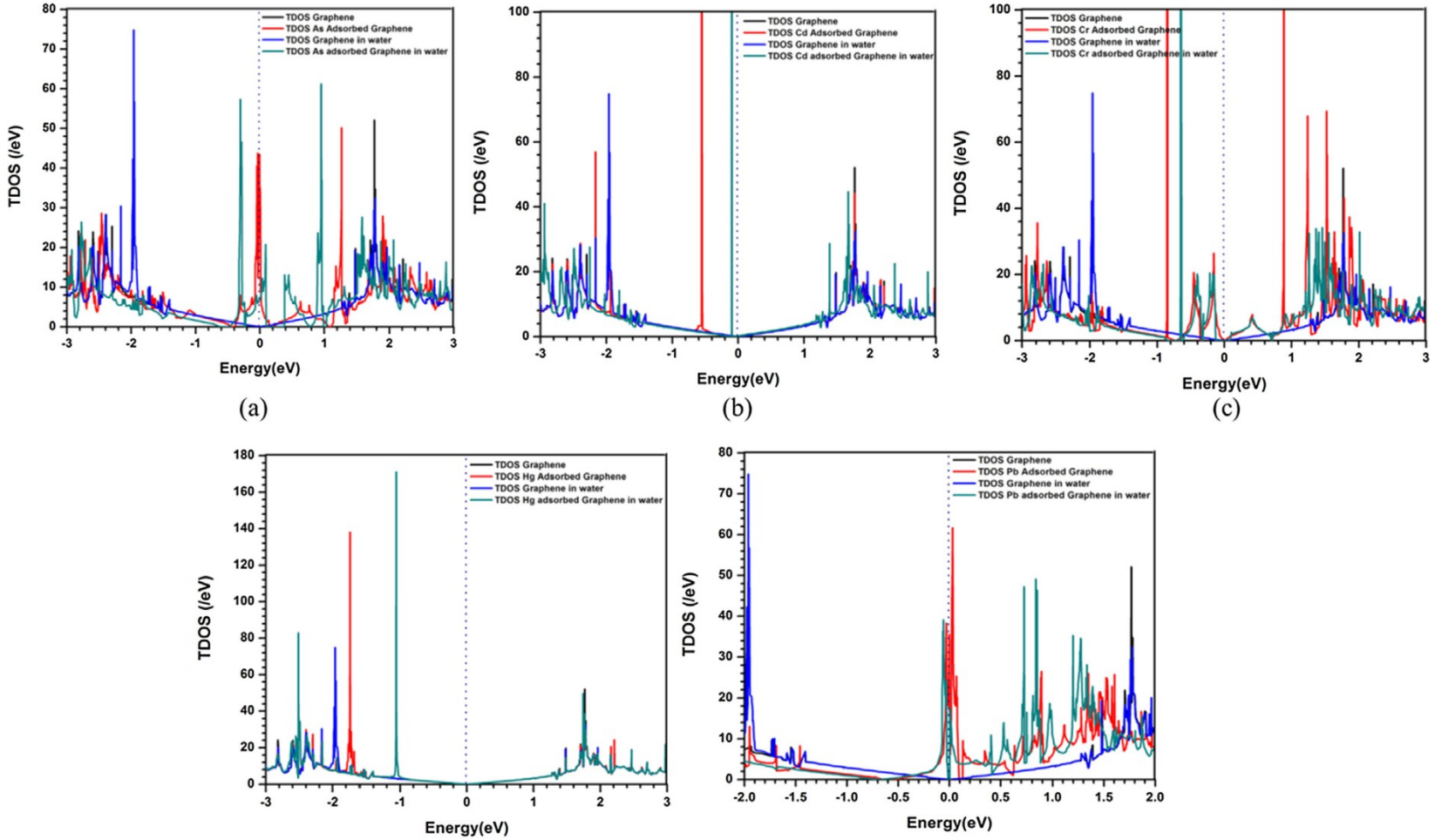
Electronic Band Structure Analysis



Band structure of graphene after adsorption of (a) As, (b) Cd, (c) Cr, (d) Hg, (e) Pb in Water environment

M. Srivastava et al, Appl. Surf. Sci. 517 (2020) 146021. doi:10.1016/j.apsusc.2020.146021

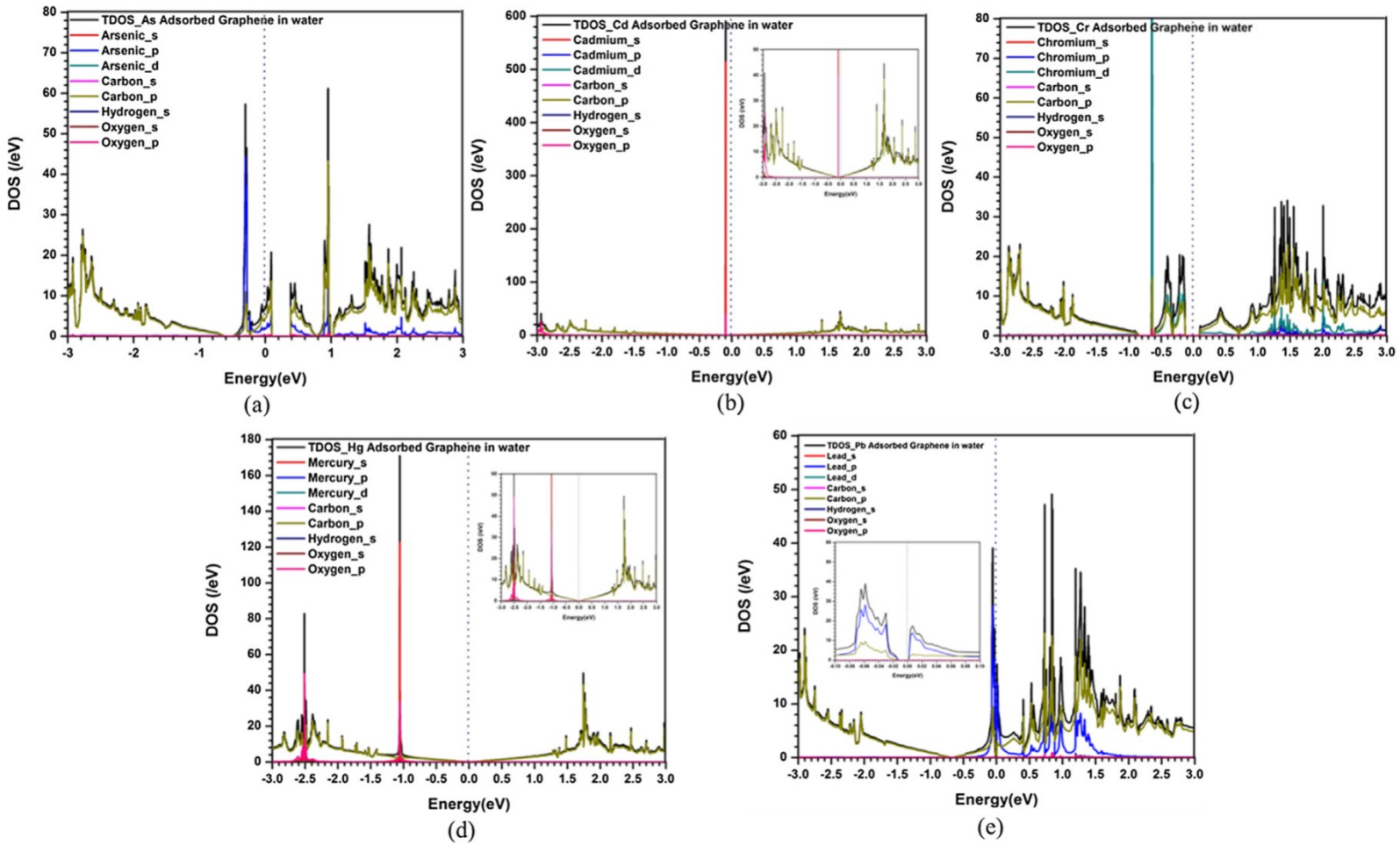
Comparison of Density of states in Vacuum and Aqueous Environment



Comparison of Density of states of graphene before and after adsorption of (a) As, (b) Cd, (c) Cr, (d) Hg, (e) Pb in Vaccum and Water environment

M. Srivastava et al, Appl. Surf. Sci. 517 (2020) 146021. doi:10.1016/j.apsusc.2020.146021

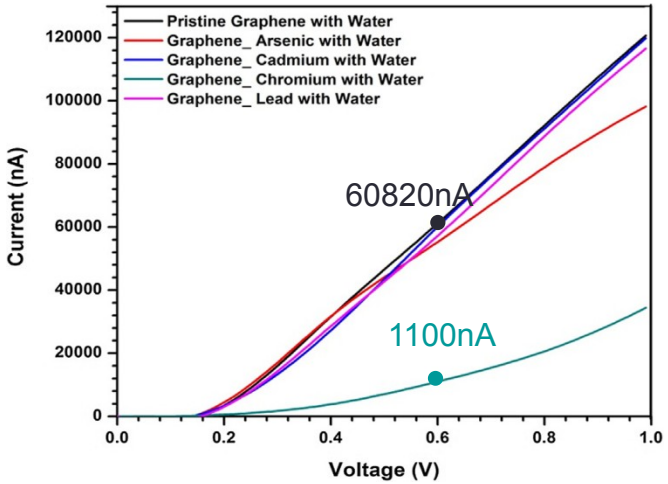
Partial Density of states profiles of the system



PDOS of Graphene sheet after adsorption of Heavy metals (a) As, (b) Cd, (c) Cr, (d) Hg, (e) Pb in Water environment

M. Srivastava et al, Appl. Surf. Sci. 517 (2020) 146021. doi:10.1016/j.apsusc.2020.146021

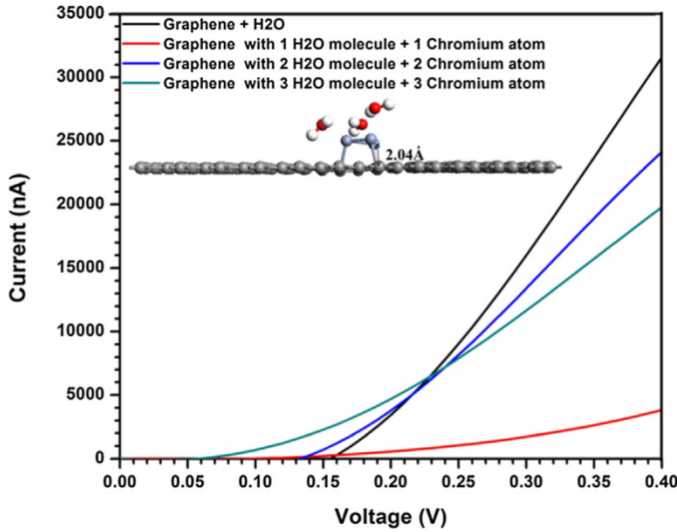
Electron Transport in Heavy metal adsorbed Graphene in Water



Current- Voltage plot for graphene sheet for the heavy metals in the Water environment.

System	Response (%)
Chromium	82% at 600mV

How Coverage Effect of Heavy metal Chromium affect the sensing performance of the device



Improvised Parameters	
Detection Range	Increases 1.54 Å to 2.04Å
Threshold voltage	Decreases by 70mV

M. Srivastava et al, Appl. Surf. Sci. 517 (2020) 146021. doi:10.1016/j.apsusc.2020.146021

Environment Protection Act

The Environment (Protection) Act was enacted in 1986 with the objective of providing for the protection and improvement of the environment. It empowers the Central Government to establish authorities [under section 3(3)] charged with the mandate of preventing environmental pollution in all its forms and to tackle specific environmental problems that are peculiar to different parts of the country. The Act was last amended in 1991

- The Environment (Protection) Act, 1986 authorizes the central government to protect and improve environmental quality, control and reduce pollution from all sources, and prohibit or restrict the setting and /or operation of any industrial facility on environmental grounds. The Environment (Protection) Act was enacted in 1986 with the objective of providing for the protection and improvement of the environment. It empowers the Central Government to establish authorities charged with the mandate of preventing environmental pollution in all its forms and to tackle specific environmental problems that are peculiar to different parts of the country. The Act was last amended in 1991.
- The Environment (Protection) Rules lay down procedures for setting standards of emission or discharge of environmental pollutants.

Environment Protection Act

- The objective of Hazardous Waste (Management and Handling) Rules, 1989 is to control the generation, collection, treatment, import, storage, and handling of hazardous waste.
- The Manufacture, Storage, and Import of Hazardous Rules define the terms used in this context, and sets up an authority to inspect, once a year, the industrial activity connected with hazardous chemicals and isolated storage facilities.
- The Manufacture, Use, Import, Export, and Storage of hazardous Micro-organisms/ Genetically Engineered Organisms or Cells Rules,1989 were introduced with a view to protect the environment, nature, and health, in connection with the application of gene technology and micro-organisms.

National Forest policies

- India is one of the few countries which has a forest policy since 1894 which was revised time to time in 1952 and 1988.
- Its aims are:
  - Maintenance of environmental stability" through preservation and restoration of ecological balance.
  - Conservation of natural heritage.
  - Checking soil erosion and denudation in catchment areas of rivers, lakes and reservoirs.
  - Checking extension of sand dunes in desert areas of Rajasthan and along coastal tracts.
  - Substantially increasing forest/tree cover through massive afforestation and social forestry programs.
  - Taking steps to meet requirements of fuel, wood, fodder, minor forest produce, soil and timber of rural and tribal populations;
  - Increasing productivity of forests to meet national needs;
  - Encouraging efficient utilization of forest produce and optimum substitution of wood; and
  - Taking steps to create massive people's movement with the involvement of women to achieve the objectives and minimize pressure on existing forests.

Wildlife Protection Act

- The act provides for the protection of wild animals, birds and plants and matters connected with them, with a view to ensuring the ecological and environmental security of India. The act constitutes a National Board for Wildlife that provides guidelines for framing policies and advising Central and State Government on promotion of wildlife conservation and controlling poaching and illegal trade of wildlife and its products;Making recommendations for setting up and managing national parks, sanctuaries and other protected areas; and Suggesting measures for improvement of wildlife conservation. It also sets up National Tiger Conservation Authority. The acts sets up various provisions related to trade and penalties for hunting the animals in wild.
- Five kinds of protected areas can be notified in the Act. These are:
  - ***Sanctuaries***- The State or Central Government may by notification declare its intention to constitute any area as a sanctuary for protecting wildlife and the environment. The government determines the nature and extent of rights of persons in or over the land within the sanctuary.
  - ***National Parks***: The State or Central Government may declare an area, whether inside a sanctuary or not, as a national park for the purpose of protecting and developing wildlife and its environment. The State Government cannot alter the boundaries of a national park except on the recommendation of the National Board for Wildlife. No grazing is allowed inside a national park. All provisions applicable to a sanctuary are also applicable to a national park.
  - ***Conservation Reserves-*** The State Government after consultations with local communities can declare any area owned by the Government, particularly areas adjacent to national parks or sanctuaries, as conservation reserves. The government constitutes a Conservation Reserve Management Committee to manage and conserve the conservation reserve.
  - ***Community Reserves-*** The State Government can, in consultation with the community or an individual who have volunteered to conserve wildlife, declare any private or community land as community reserve. A Community Reserve Management Committee shall be constituted by State Government for conserving and managing the reserve.
  - ***Tiger Reserve-*** These areas were reserved for protection tiger in the country. The State Government on the recommendation of the Tiger Conservation Authority may notify an area as a tiger reserve, for which it has to prepare a Tiger Conservation Plan.