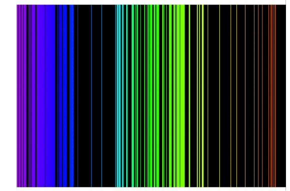
THE OHIO STATE UNIVERSITY

Ohio Supercomputer Center



Research based online course:

"Atomic and Molecular Astrophysics and Spectroscopy with Computational workshops on R-matrix and SUPERSTRUCTURE Codes I"

- PROF. SULTANA N. NAHAR,
PROF. ANIL K. PRADHAN
Astronomy Department, Ohio State University, USA

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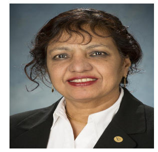
A.P.J. Abdul Kalam STEM-ER Center
(Indo-US collaboration)

- Organized under the Indo-US STEM Education and Research Center of OSU-AMU, AMU, Aligarh, India, & OSU, Columbus, USA

May 4 30, 2024

Support: OSU-AMU STEM ER Center, AMU, OSU, OSC



Research training based course on "Atomic and Molecular Astrophysics and Spectroscopy with computational workshops on the R-matrix, SUPERSTRUCTURE codes" being offered under the Indo-US APJ Abdul Kalam STEM Education and Research Center of Ohio State University (OSU)-Aligarh Muslim University (AMU), by Prof. Sultana N. Nahar (Email: nahar.1@osu.edu) jointly with Prof. Anil K. Pradhan (AKP, pradhan.1@osu.edu), Dept of Astronomy, OSU, USA

- Lectures & Workshops: 4 weeks, Saturdays & Sundays, 3 hours/session, May 4 - 30, 2024
- Venue: online zoom platform. Time: 11 am - 2 pm, US Eastern time
- Computational Facility (online): Ohio Supercomputer Center (OSC), USA

Course certificates (completion/participation w/o exam) will be provided, participation is free

- Textbook: "Atomic Astrophysics and Spectroscopy" -By A.K. Pradhan and S.N. Nahar (Cambridge University Press, 2011)
- Contacts: Prof. Tauheed Ahmad, Director, Indo-US STEM Education and Research Center, AMU, India Email: ahmadtauheed@rediffmail.com, Mobile: 91-8279632366, 9837404077

SYLLABUS

Week 1 (May 4,5, 2024): *Plasma, Atomic Structure, Computational Workshop*

i) Light and Matter, Plasma Sources, Particle and Photon Distributions, Overview on Applications (AKP): Chemical abundances, exoplanetary atmospheres, opacities, nano-biomedical X-rays. etc.
ii) Atomic Structure: Hydrogenic & Non-Hydrogenic Spectra
iii) Hartree-Fock, Dirac, Breit-Pauli Approximations
iv) Computational Workshop: SUPERSTRUCTURE

Week 2 (May 11,12): *Radiative & Collision processes, Computational Workshop*

i) Atomic Process in Plasmas - Radiative Transitions, Electron-Impact Excitation (EIE),
ii) Photoionization, Electron-Ion Recombination
iii) Close-Coupling Approximation and R-matrix Method
iv) Computational Workshop: SUPERSTRUCTURE

Week 3 (May 18,19 2024): ***Computational Workshop on EIE using R-matrix codes, Molecular Structure & Spectra***

i) Electron-Impact Excitation
ii) Line Ratios for Plasma Diagnostics
iii) Computational Workshop: R-matrix Calculations for EIE
iv) Prof. Pradhan lecture: Molecular Structure and Astrophysical Spectra

Week 4 (May 25,26, 2024): ***Astrophysical Applications, Exam, Certificate***

Prof. Anil Pradhan's lectures: i) Plasma modelling and Plasma opacity
ii) Review of materials
iii) Exam and evaluation
iv) Preparation and distribution of Certificates by May 30, 2024
NOTE: Computational workshops on R-matirx method are divided in two parts
- Part I: Collisional excitation and Part II: radiative processes
• Present form: Part I: Focus will be on Electron Impact Excitation

GLOBAL PARTICIPATION REGISTRATION:

• To enroll, email the following information (the way you want for the certificate)

Full official name:
Designation (Prof, Dr., Researcher, Student with current status of education):
Name of the affiliated University or Institution:
City and country names:
Email:

• zoom link for the sessions:
https://osu.zoom.us/my/snnahar?pwd=TkJvNnptTzRQSEZ4c3RWNzBDV2pSZz09
Personal meeting id: 665 664 7991, pw: 330775

• Please create your account at Ohio Supercomputer Center (OSC) following the instructions in the next pages. Note: OSC will provide a new access code.

Get your account at Ohio Supercomputer Center (OSC)

For the computational workshops, you will need an account at OSC. Please follow the steps below from the weblink
- https://www.osc.edu/supercomputing/portals/client_portal/self_signup_for_account
- Click on blue highlighted link "MyOSC" right below "Self-Signup for Accounts

It will open up to a window for "log in" and "Sign-up". For new account click on "Sign-up" which will open up "Your Contact Information" page

Enter your information (Red asterisk boxes).

If you do not have institutional email address, put down the email address that you have. Click on the "Submission" bar.

OSC will send you an email with a code to verify your email address and open a window to type that code. So check your email to get the code and put it in the box "Enter your Code here". - Click in the box "I'm not a robot". You get a CAPTCHA image to click on boxes

This will go to the next page with you will enter your access code:
- Project code: PAS1866
- Access code: 635858

NOTE: We will recieve a new access code on May 14.

- To login to your account, you will go to the same page of "myosc portal". Please remember to use Project code and the Access
- To log in to you account from a "terminal window". Follow as:

- Type: ssh YourID@owens.osc.edu (ssh app could already be in your computer)
- or: ssh -o serveraliveinterval=60 YourID@owens.osc.edu

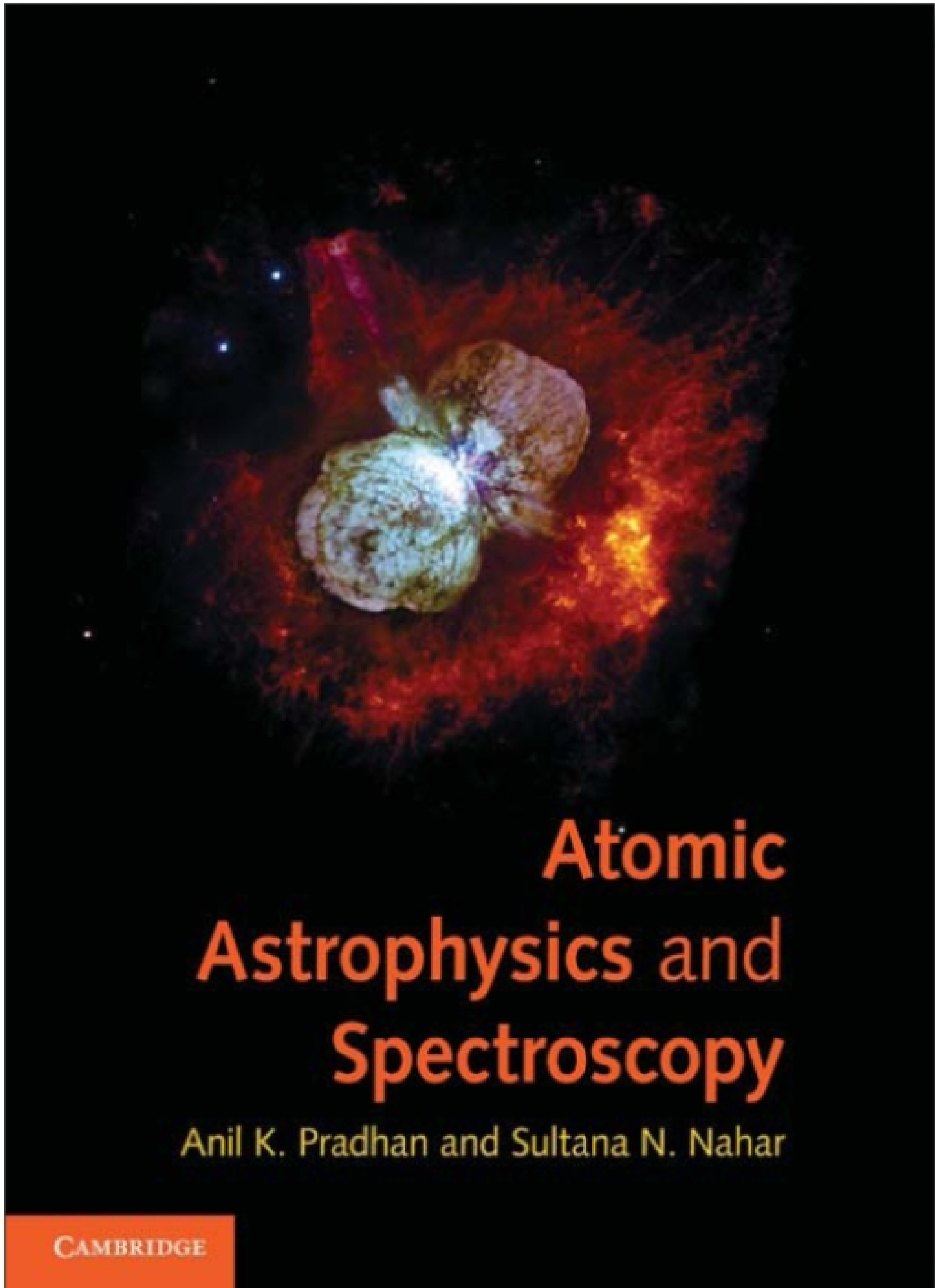
The option "-o serveraliveinterval=60" lets you stay logged in for a longer time.
Please note that after typing each command, you will hit the <return> key

Log in to you OSC account for running jobs

For the computational workshops, you will need a terminal window where you can write commands for viewing and editing files, submitting and running programs. You can use any of the following terminals:
- i) The terminal window that exists in your computer
- ii) Download from the internet "Putty" which creates a terminal window to log in to a remote host
- iii) use the terminal window that OSC provides from "onDemand" log in page. For the OSC terminal, please follow the steps below:

• On the internet, go to: https://ondemand.osc.edu
• Click on "OSC OnDemand - Ohio Supercomputer Center"
- OSC log in page will open up.
• Type in your user name and password and click on the bar stating "Log in with your OSC account"
- You will be led to your account page
• From the top blue bar, click on the "Clusters" and drag your cursor to "Owens shell access".
- This will take you to the terminal window to work (black background)
• Work on your programs: copying, running, check the input output files etc.
• When done with your work, go to the previous page by clicking on the "Dashboard OSC" box at the top bar of your browser
• On the right of the top bar on you account page, you will find "log out" to click and get out.
• For any issue, contact OSC at: oschelp@osc.edu
Can also communicate to Heidi Hamblin at: hhamblin@osc.edu

- Download the book from free websites



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Invite to APS membership:

AMERICAN PHYSICAL SOCIETY (APS)

- It is the largest scientific network for physics and related subjects.
- APS journals are Phys. Rev. A, B, C, D, E, PhysRevLett, etc.
- It holds two general and quite a number of conferences every year
- It gives many prestigious prizes and awards, and a number of grants
- APS Membership can be free for 4 - 6 years and be renewed for developing countries, free for 1 year for any US/non-US student:

Website: http://www.astronomy.ohio-state.edu/~nahar/fip.html

- From "APS MEMBERSHIP" information, download the Application form, fill it out, and send it with your CV at the email address given at the website. You will hear from APS in a week.
- After becoming member (will receive ID from APS),

\- Get your web account using your account
\- become a member of your division & of APS unit - FIP: Forum of International Physics
\- Post your resume
\- Sign up for job alerts and apply online
\- Submit abstracts for APS conferences
\- Check many other activities and benefits, such as,
free issues of Physics today, newsletters, calendar, research alters, application notices for various recognition

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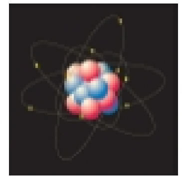
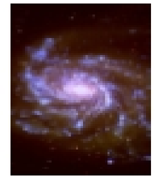
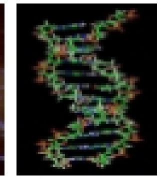
    

INTERNATIONAL SOCIETY OF MUSLIM WOMEN IN SCIENCE (ISMWS)

ISMWS CHARTER

Founder: Dr. Sultana N. Nahar
The Ohio State University, Columbus, Ohio, USA
April 19, 2010

- **AIM:** - encourage Muslim women in science profession, form a network for various support
- **Objective:** Stay in Science (basic or applied)
- **Motto:** Out of 24 hours a day, we keep some hours for our intellectual nourishment
- **Members:** Over 400 from 32 countries & has chapters

Web: http://www.astronomy.ohio-state.edu/ ~nahar/ismws.html

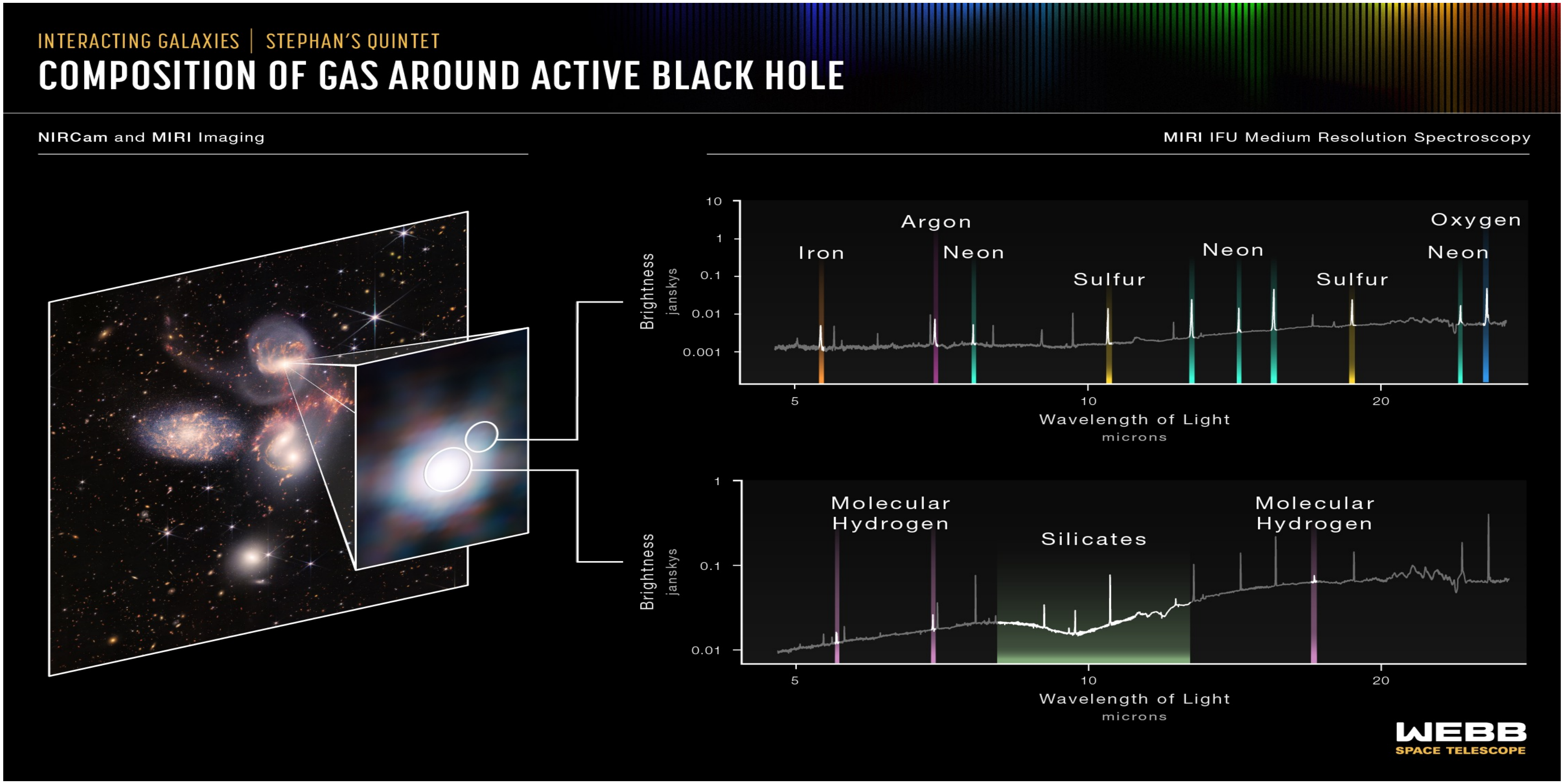
For membership (free) - Email: nahar.1@osu.edu

Near empty space: Spiral galaxy NGC 3521 Ours: MILKY WAY

• There are about 2 trillion galaxies in the observable universe. Before Hubble's finding, the Milky Way was assumed to be the whole universe.
It is important to study the space & we have a long way to go

• Observable universe size: about 93 billion light years. How do we study the universe? - Through atomic & molecular spectroscopy

Light and Matter: **SPECTRA OF A BLACKHOLE MEASURED BY JWST**

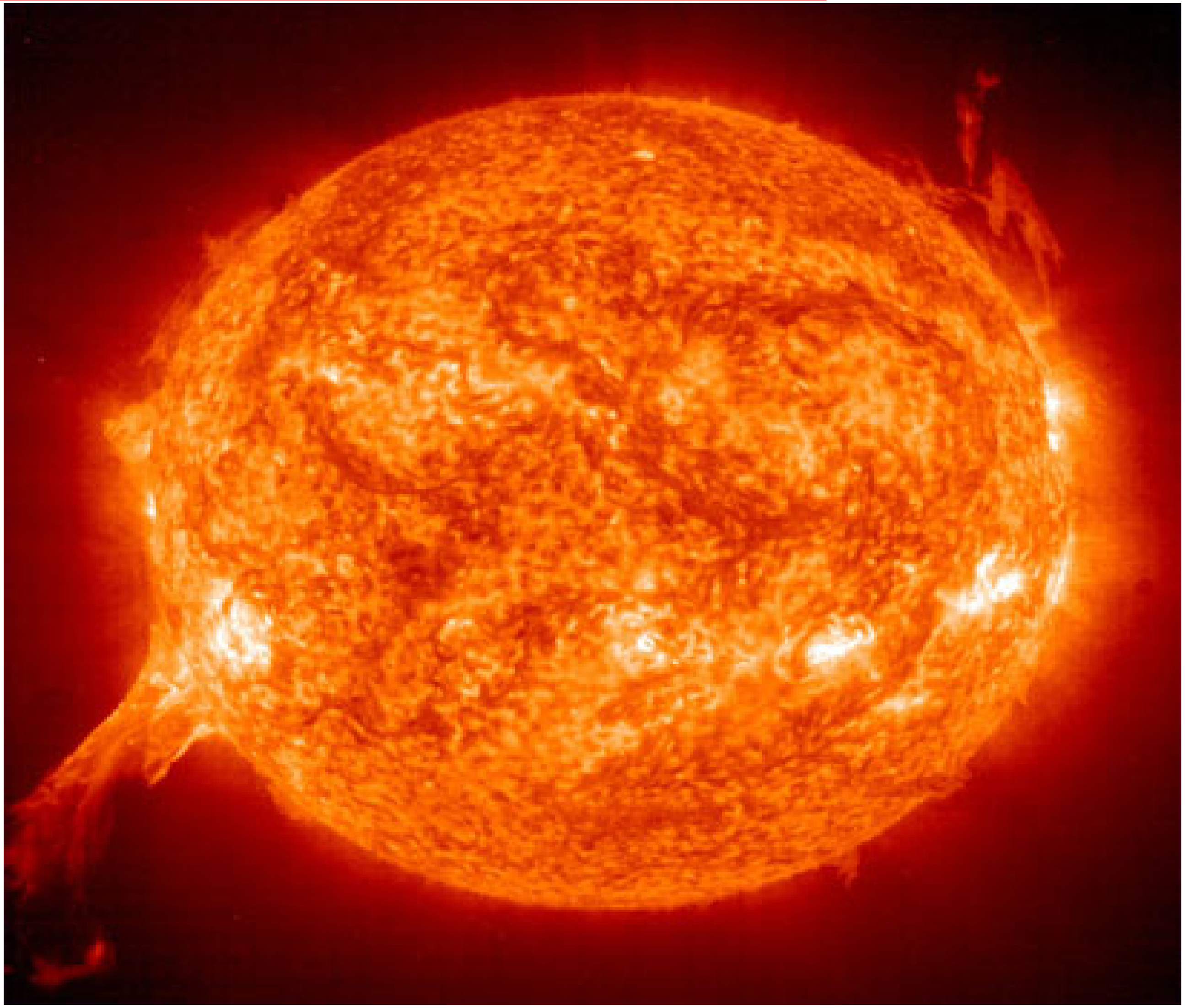


The MIRI (Mid-Infrared Instrument) instrument measured the composition of gas around the black hole at the center of one of the galaxies in Stephan's Quintet. • It found a region filled with hot, ionized gases, including iron, argon, neon, sulfur and oxygen (top spectrum). • The instrument also revealed that the supermassive black hole has a reservoir of colder, denser gas with large quantities of molecular hydrogen and silicate dust (bottom spectrum).

ASTRONOMY: Anything beyond our earth - but important to study. Our galaxy: MILKY WAY (stable)

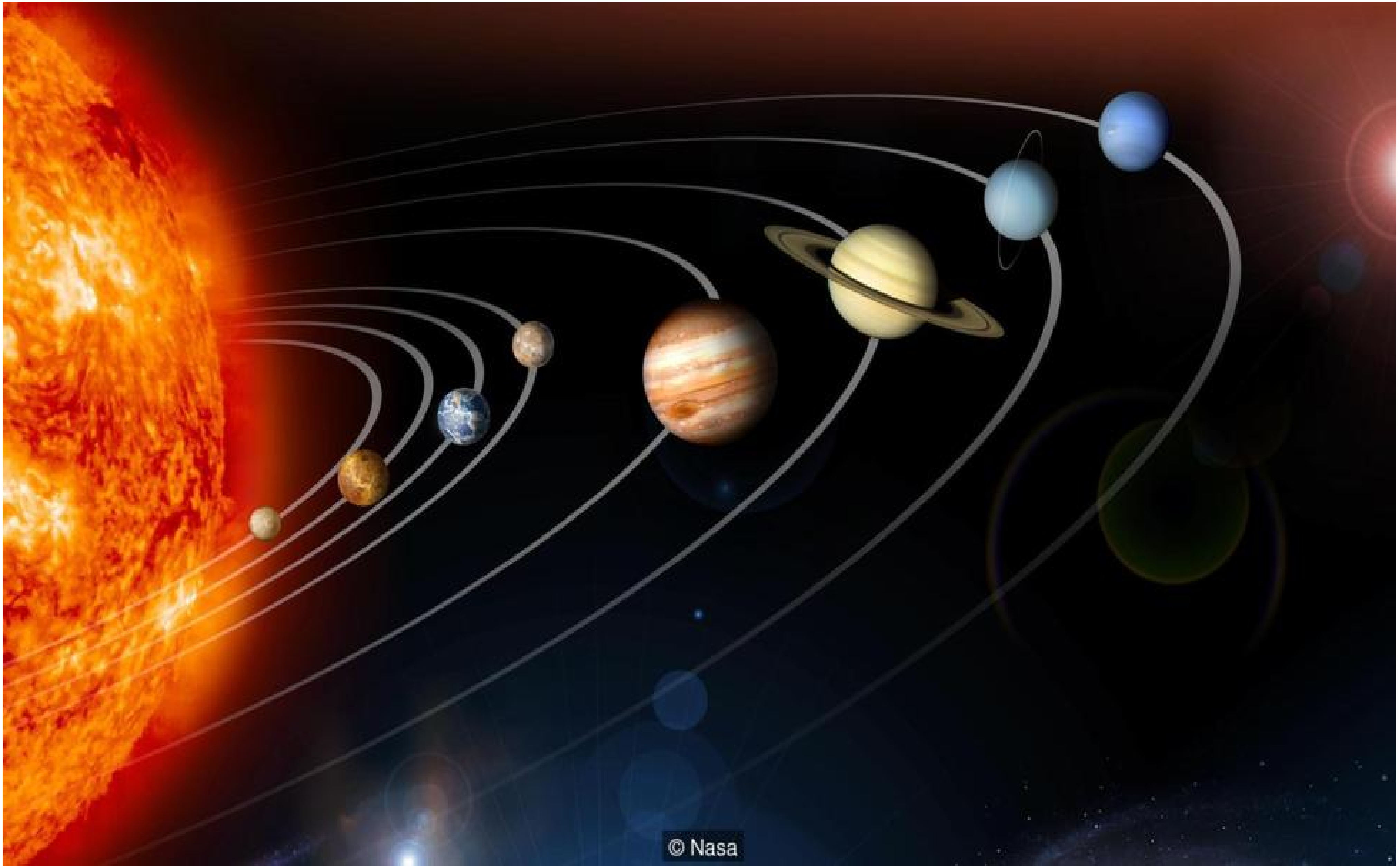
• Has 200-400 billion stars. About 98% of the stars will lead a life evolution similar to the Sun. • Milky way is spherical. Crossing over will take (diameter) over 100,000 LY. The Sun is near the edge of it Light or radiation is emitted by excited or "HOT" atoms, molecules in them Being near edge it avoids risk of being swallowed by a BH.

OUR SUN - The "unQuiet" Star (Observed by SOHO)



- The Sun - a very dense and hot ball of plasmas
- Sun has a 11 years cycle of minimum to maximum ACTIVITY, when its magnetic field flips between North & South. Pic: White active magnetic regions & flares on the surface. A typical solar flare ~ larger than the earth • Activity: Eruptions with explosions & ejecting large amount of particles & radiation in to space which can affect the earth

The SUN, our STAR (diameter: 110 x Diameter-earth)

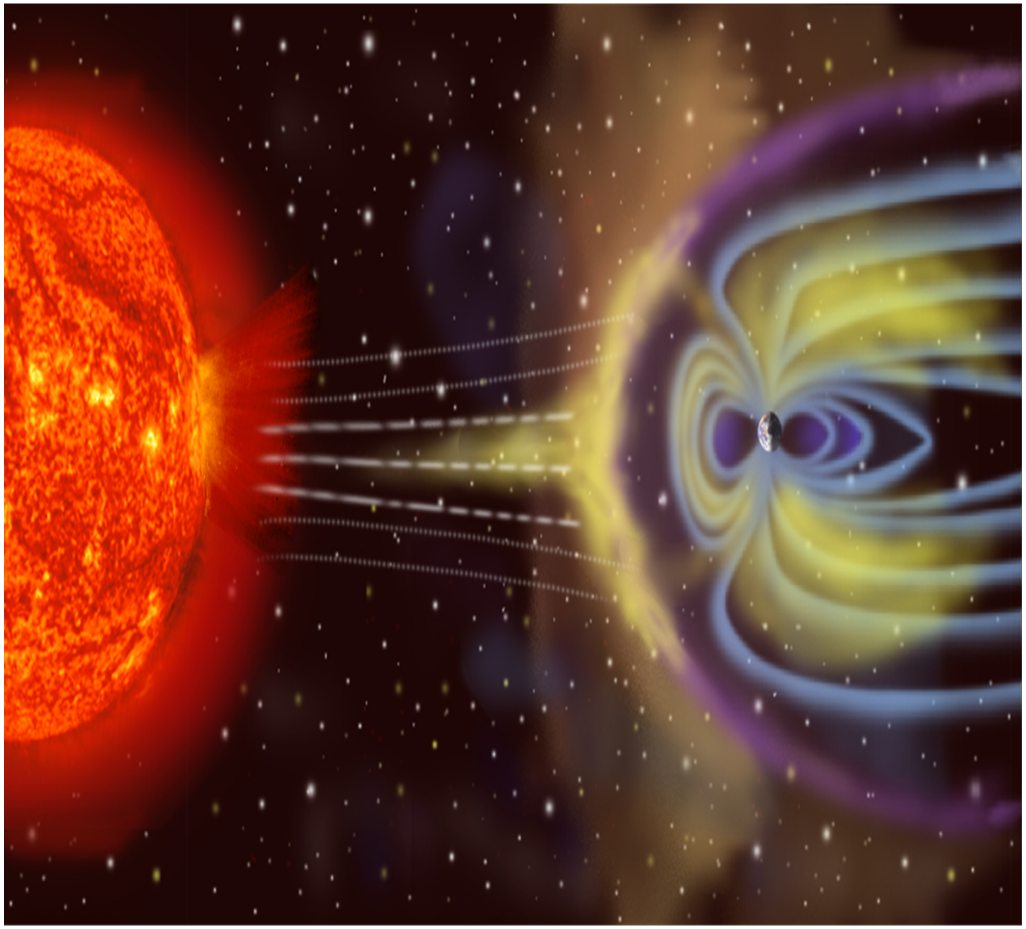


- **The Sun has 8 planets (M-V-E-M terrestrial, J-S-U-N gaseous)**
- **It is an extremely dense and hot ball of plasma, gives out huge amount of radiation, Only small fraction of sun's radiation reaches the**

The EARTH: Our beautiful home

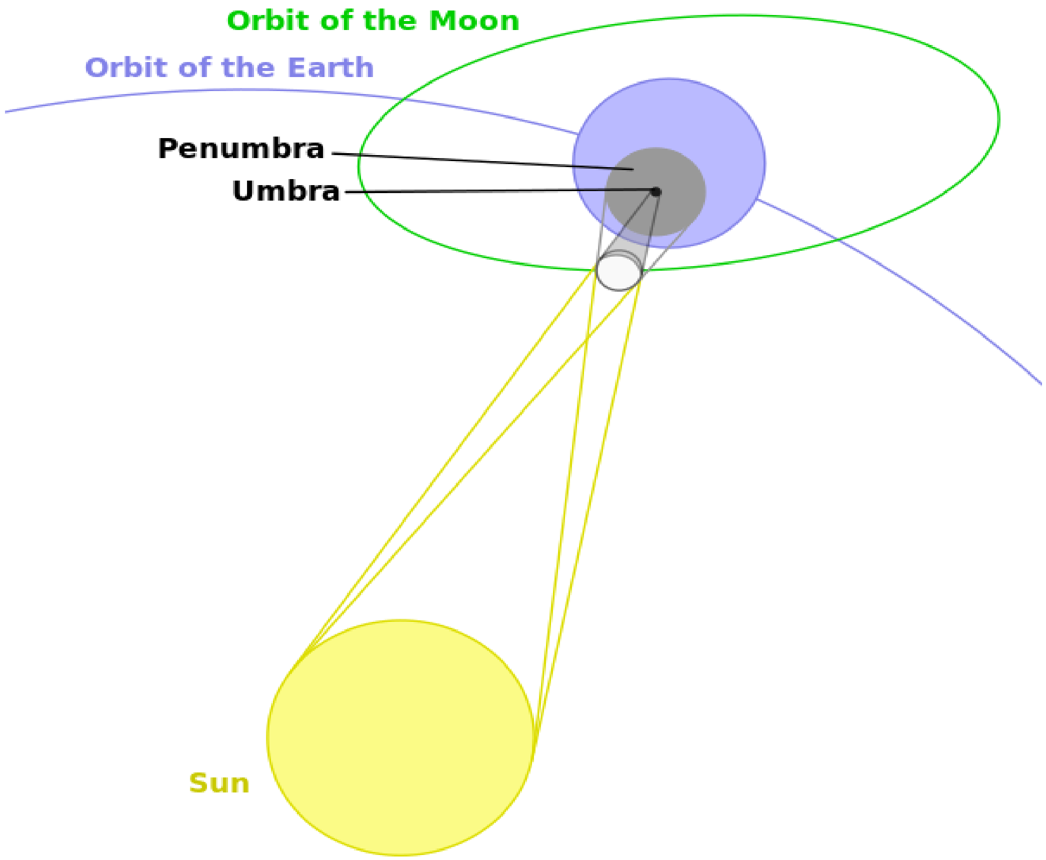
- Sky is blue at high Sun because atmospheric molecules scatter the blue photons to the earth. Blue sky is reflected on the water.
- Sunrise or sunset brings red photons as they travel through layers of atmosphere and bend to reach earth's surface. This also causes Sun to be seen when it may be below the horizon

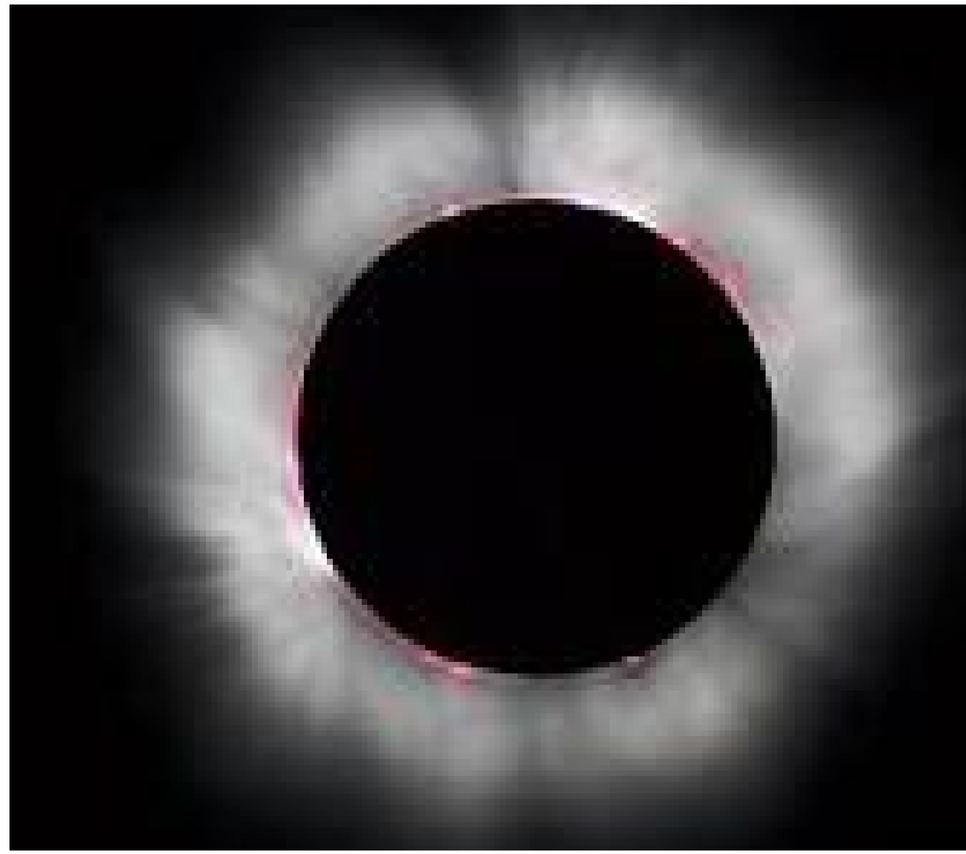
The SUN has Solar Storms: Ejects Radiation & Particles



- The active sun with solar spots blasts huge amount of radiation Gamma ray, x-ray, UV, and charged particles in space which are harmful to us. But we are protected:
- i) the atmosphere deflects, burns the particles, ii) ozone blocks high energy radiation, iii) its magnetic field captures the charged particles seen as aurora or the northern lights.

SOLAR ECLIPSE (April 8, 2024)



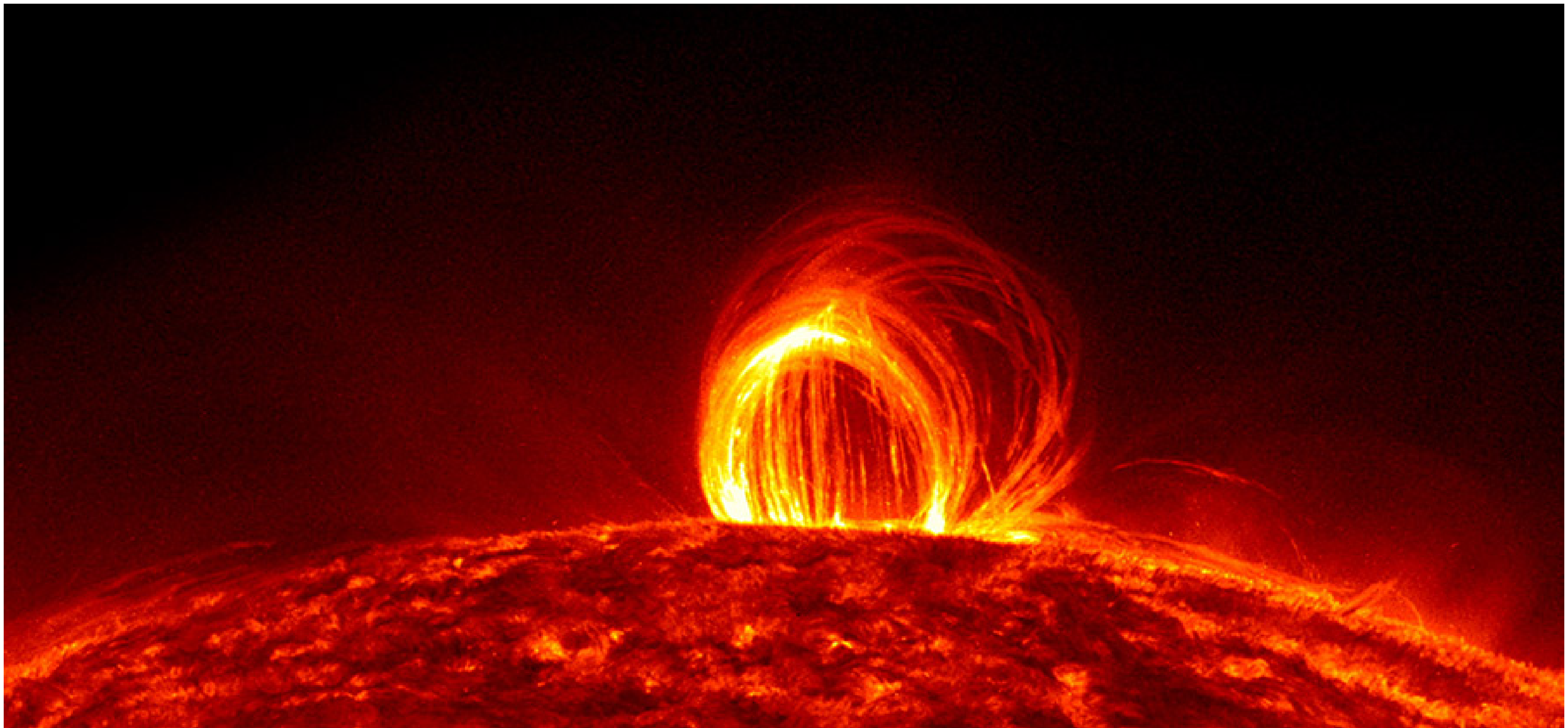


- Total solar eclipse, a cosmological event of interest, occurs at occasional alignments of the Sun, Earth and Moon. • Total eclipse gives the scope to see the surrounding of the Sun blocked by Sunlight
- The Sun is surrounded by three outer thin plasma regions: Photosphere (surface to 250 mi, 6500 - 400 K), Chromosphere (250-1300 mi, 4000 - 8000 K), Transition Region (60 mi, 8000 - 500,000 K) and the Corona (1300 - , 500,000 - a few Million K)

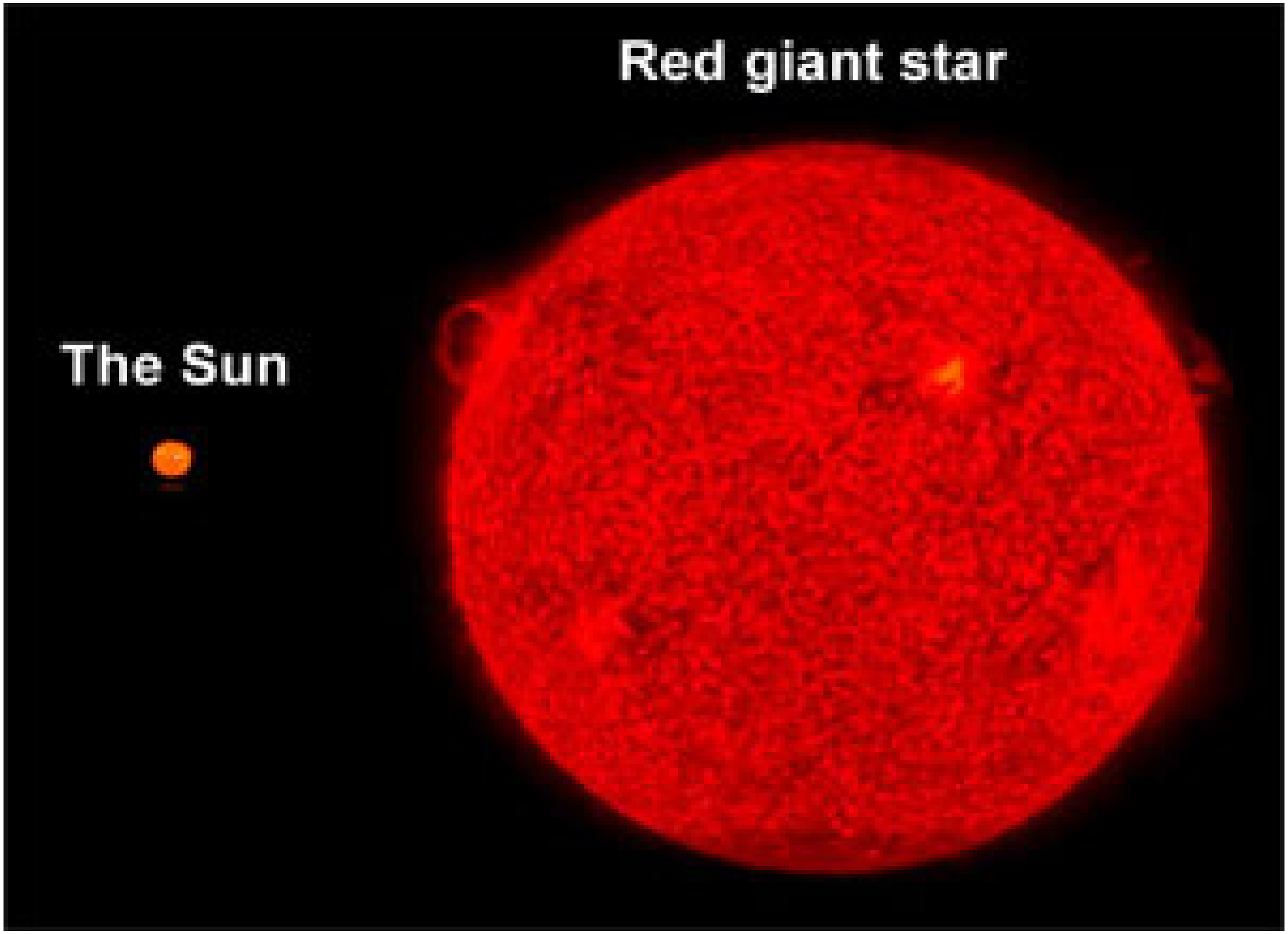
CORONAL TEMPERATURE & Fe XIII FORBIDDEN TRANSITIONS

• High temperature in corona was a mysterious finding of Edlen. The forbidden transitions within the ground ^3P state of highly charged Fe XIII was strong to be observed in solar flare by Edlen who then calculated the flare temperature over million degrees compared to the assumed value of a few thousand degrees. Sudden rise in temperature in Corona, which is much further away from the surface of the Sun, has remained a puzzle

- Physics Today (jul 2023): A new instrument reveals not only the size of plasma rain in the Sun's corona but also the atmospheric response, which provides more clues about the coronal-heating phenomenon.



LIFE OF OUR SUN: RED GIANT IN 6-7 BYR



• SUN: 4.5 BYr old, live for another 6-7 BYr. The current age of the universe $\sim$ 13.8 BYr
• It will become a Red Giant, a dying expanded star with H fuel gone
• The heat, radiation, electrons will push materials out to form a red giant. • Red giant will slowly become planetary nebulae and ultimately white dwarf. Over 90% stars will end up to white dwarf and lot of

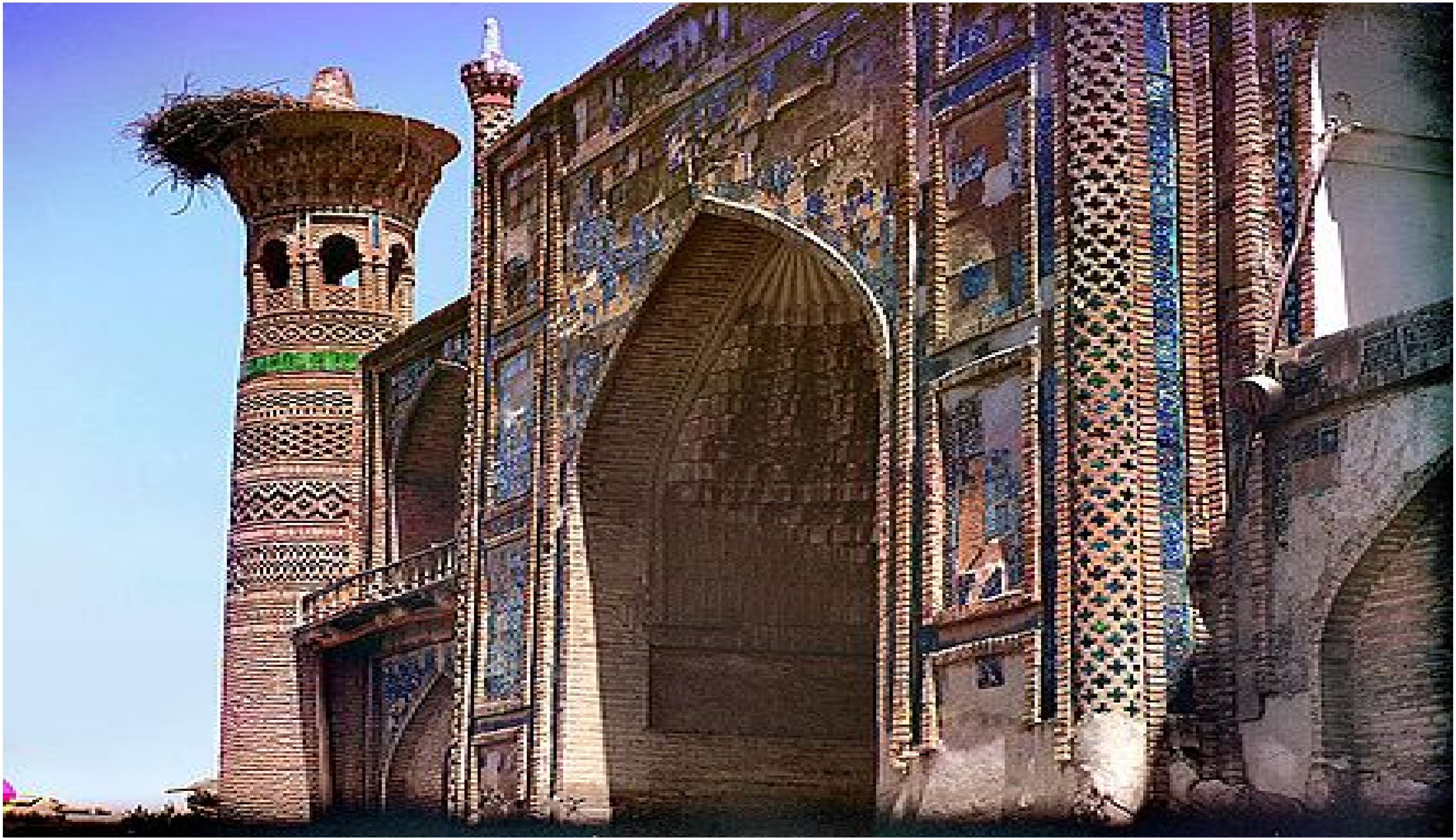
PLANETARY NEBULAE - Endpoint of a Star [PNe K 4-55 below]

- Condensed central star: very high T $\sim$ 100,000 K ($>>$ T $\leq$ 40,000 K - typical star). Envelope: thin gas radiatively ejected & illuminated by central star radiation: red (N), blue (O). Lines of low ionization states - low ρ & low T
- Ionized gaseous nebulae: associated with birth & endpoint of stellar evolution $\longrightarrow$ chemical enrichment is a chronometer of life of the universe itself

End of life: WHITE DWARF - Ex: Diamond white dwarf 2014

- "Astronomers discover Earth-sized diamond-encrusted white dwarf" 2014. It is so old that it has crystallized into a Earth-sized diamond
- A white dwarf is very dense: its mass is comparable to that of the Sun, while its volume is comparable to that of Earth.
- About 98% stars will end up as white dwarfs

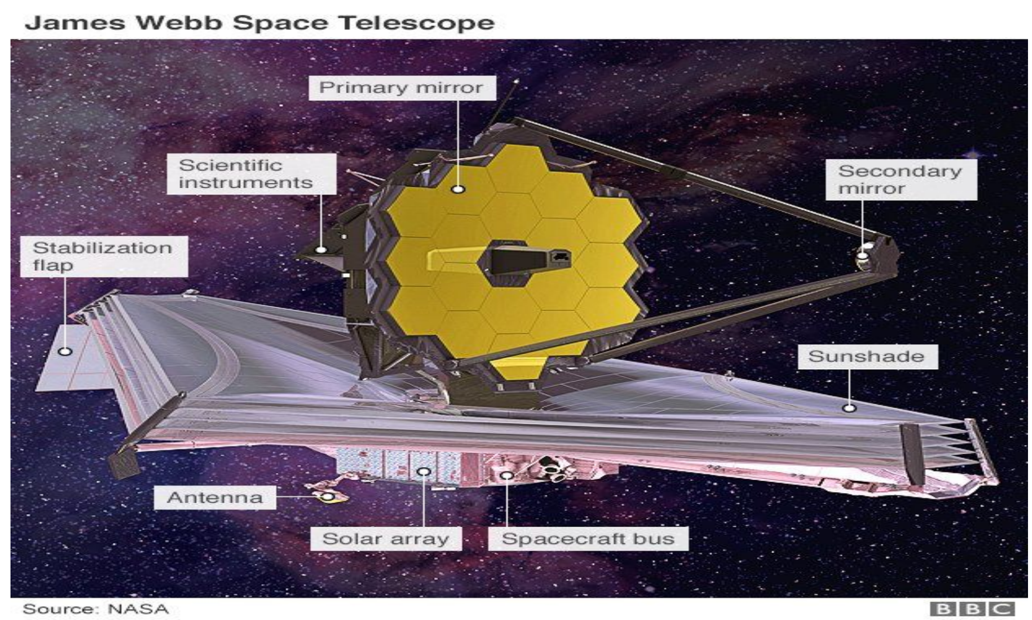
THE 1ST OBSERVATORY, SAMARKAND, 1420, BY MUSLIM RULER ULUGH BEG (Iran has an older model)



- Ulugh Beg built the madrasa in 1420 in Samarkand and extended it to an observatory
  - Beg himself recorded many astronomical objects.

MODERN DAY GROUND & SPACE BASED TELESCOPES

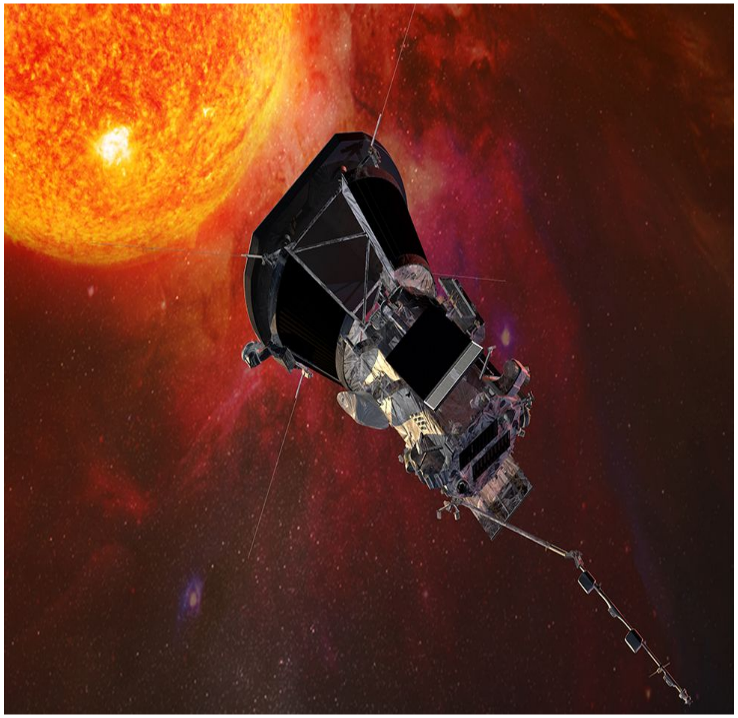
L: Large Binocular Telescope in Arizona (8.4m Mirrors, NIR-optical), R: Hubble space telescope

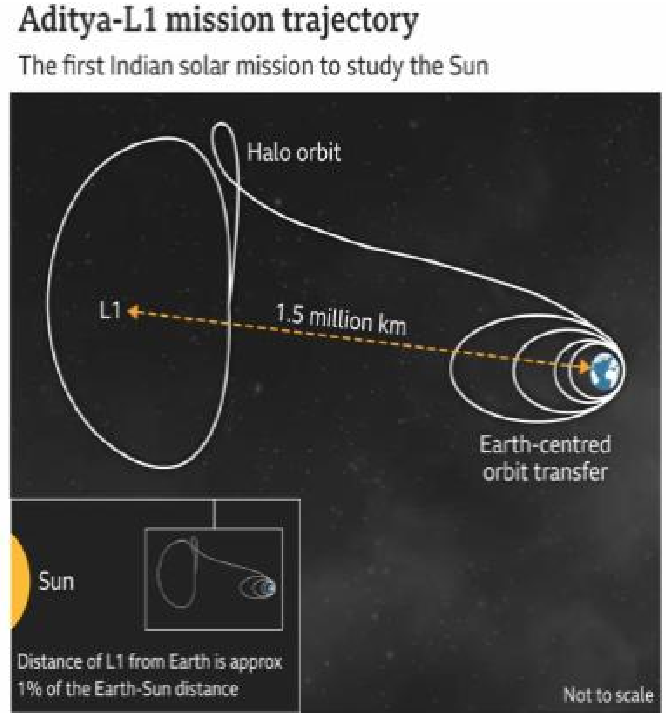


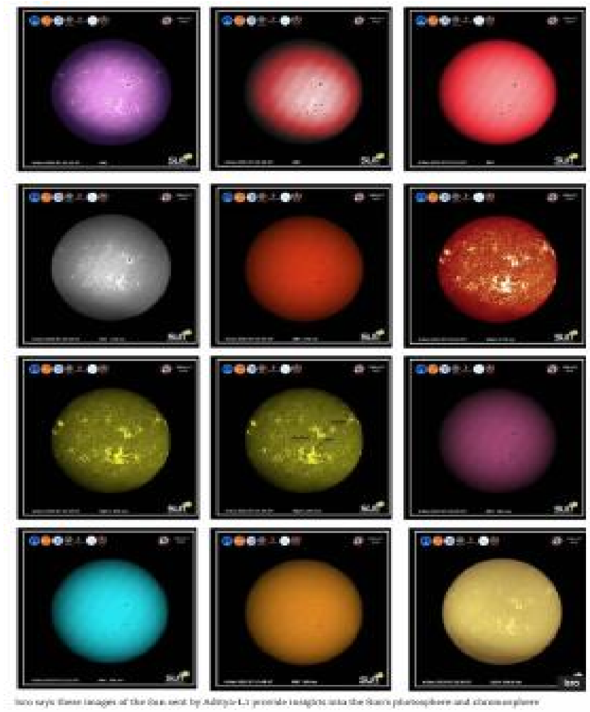
L: International Space station of NASA, R: JWST

How India's Chandrayaan-2 will reach the Moon

DEDICATED OBSERVATORIES FOR THE SUN
PARKER SOLAR PROBE & ADITYA L1

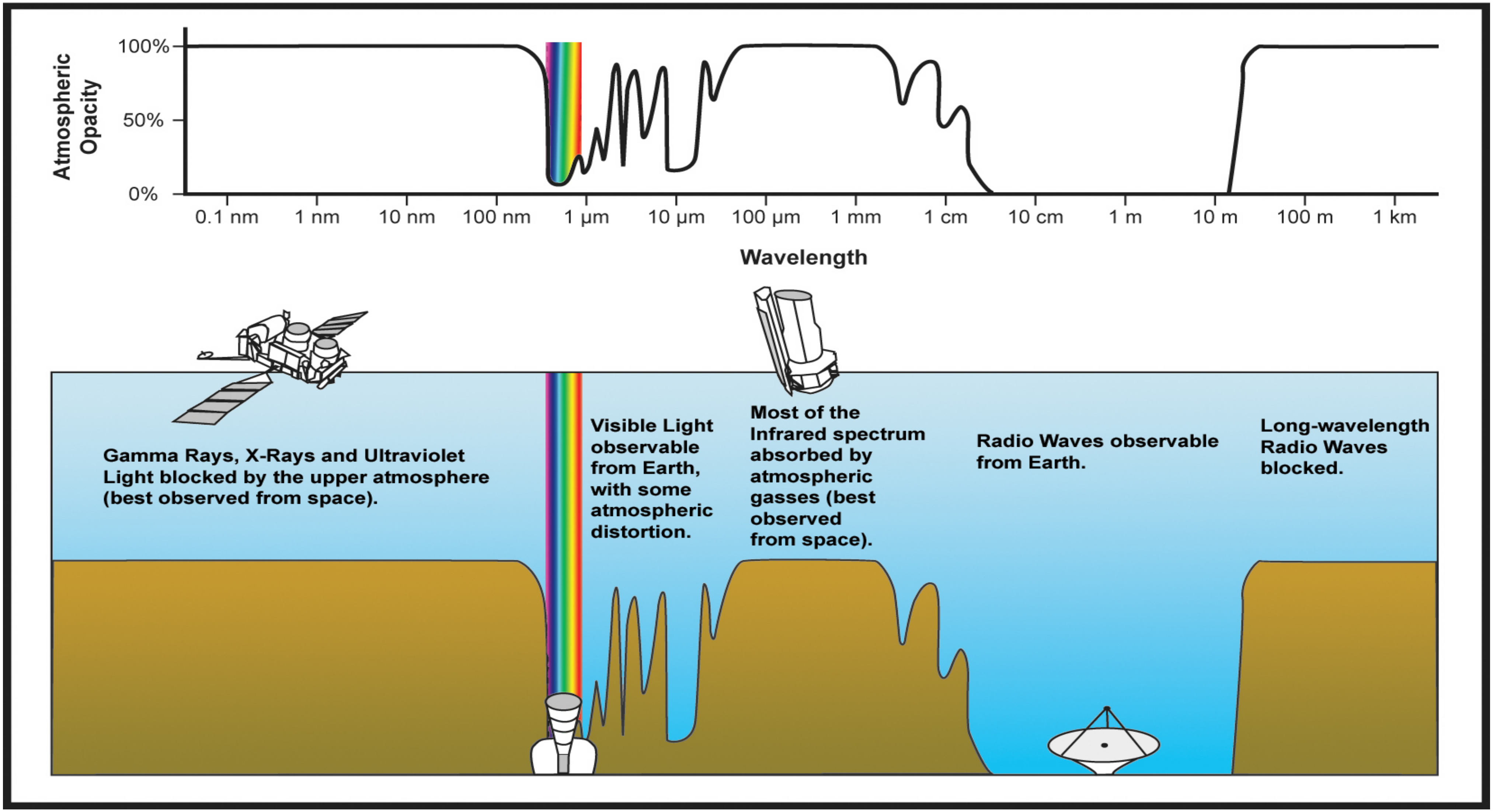






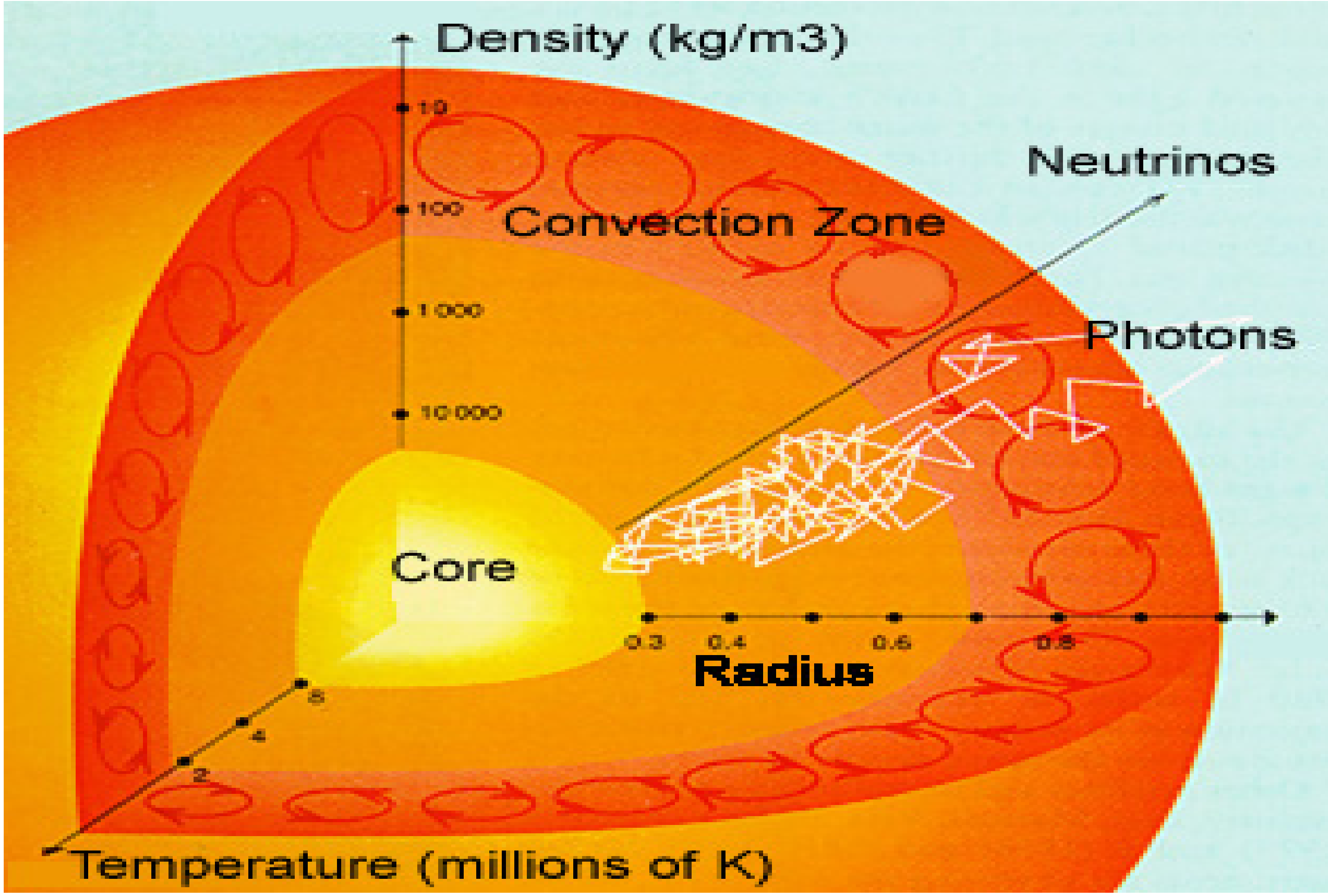
- L: Parker Solar Probe makes historic pass through Sun's atmosphere withstanding intense heat.
  - A satellite/ spacecraft goes around the earth several times, each time making a longer elliptical loop by the gravitational push, until going straight toward the object - path of Indian spacecraft Aditya L1 (Lagrange point 1) to study the Sun.
  - It sent various images of the Sun in corona and chromosphere.

ATMOSPHERIC OPACITY - ABSORPTION OF RADIATION



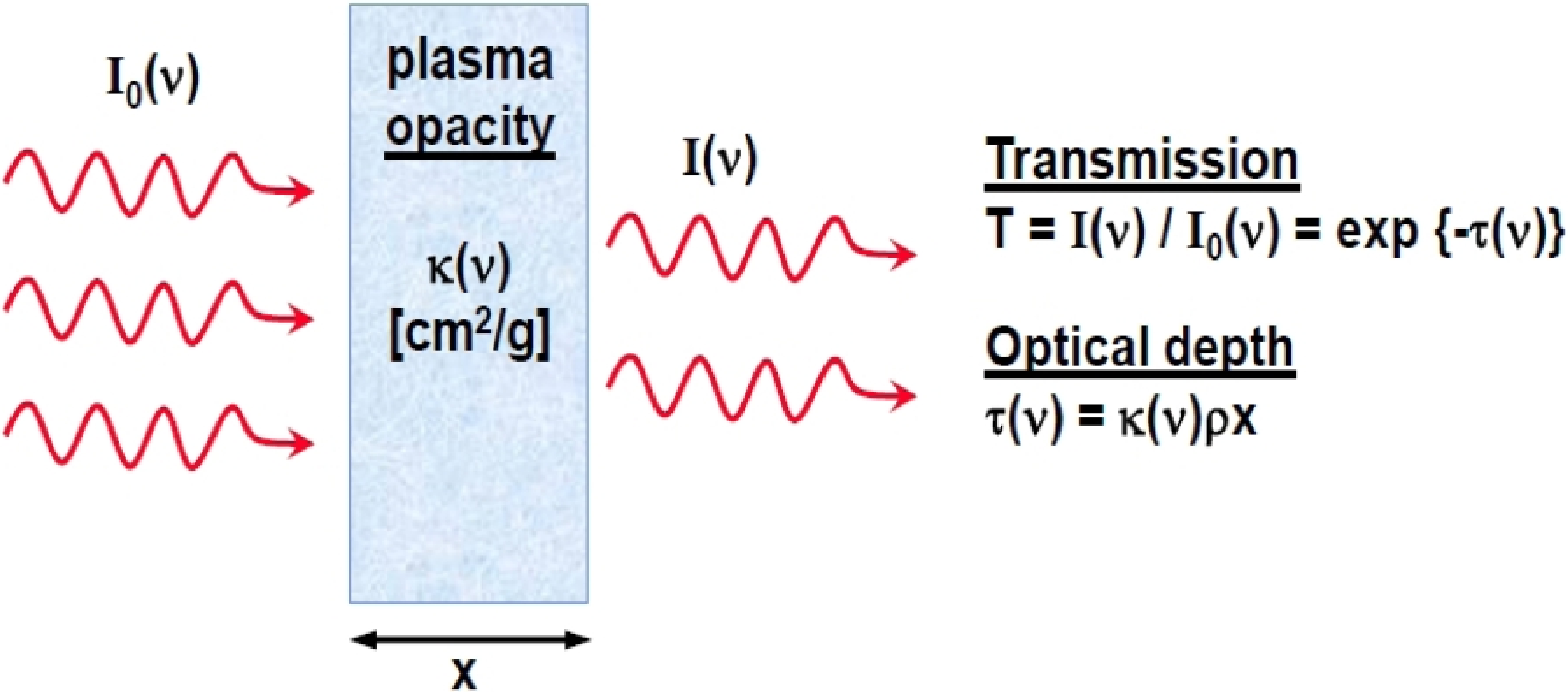
- Higher opacity -less radiation reaching earths surface
- Opacity determines types of telescopes - earth based or space based
- Gamma, X-ray, UV are blocked while visible light passes through
- CO_2, H_2O vapor, other gases absorb most of the infrared frequencies
- Part of radio frequencies is absorbed by H_2O and O_2, and part passes through

SOLAR PLASMA OPACITY & ELEMENTAL ABUNDANCES



• 3 regions of the Sun: 1) Core: 15 mK, 150 g/cm^3 - nuclear fusion center - H fuses to He & produces gamma rays, 2) Radiative zone - highly dense and hot plasma - energy transfer through diffusion, 3) Convection zone - boiling plasma. The change in phase between radiative and convection zones is distinct. The boundary distance R_{RC} is known. • Absorption of radiation by the constituent elements cause solar plasma opacity and slow down the escape of the radiation. R_{RC} can be predicted from opacity

PLASMA OPACITY



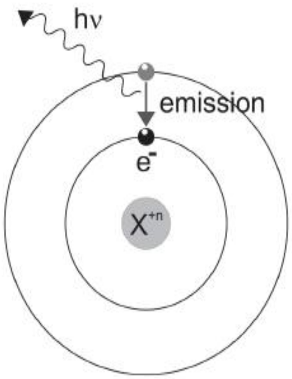
- Opacity $\kappa(\nu)$ is a fundamental quantity for radiation absorption during transmission in plasmas. Microscopically monochromatic opacity $\kappa(\nu)$ depends on two radiative processes:

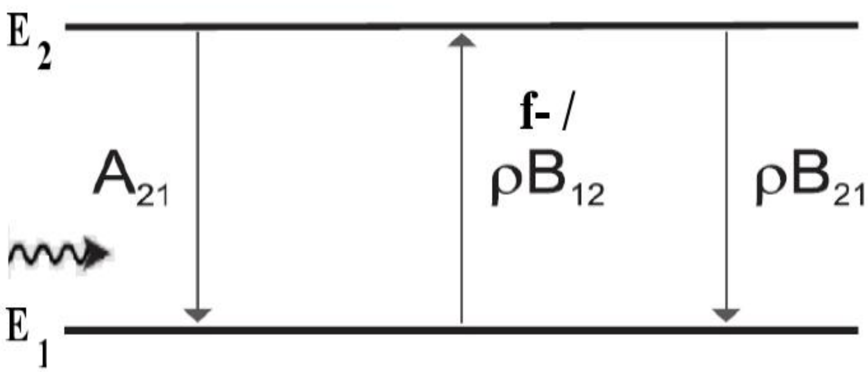
1. Photoexcitation - $\mathbf{X^{+Z} + h\nu \rightarrow X^{+Z*}}$
2. Photoionization - $\mathbf{X^{+Z} + h\nu \rightarrow X^{+Z+1} + \ e}$

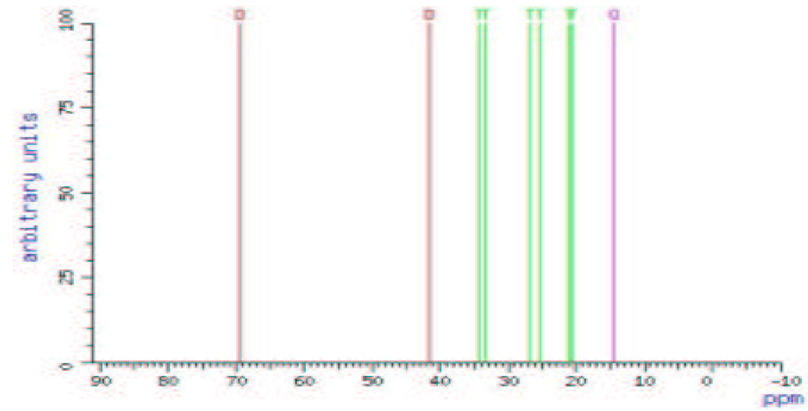
- DIFFICULTY - needs huge amount of atomic data: The total $\kappa(\nu)$ is obtained from summed contributions of all possible transitions, both bound-bound & bound-continuum, from all ionization stages of all elements in the source

Opacity: PHOTO-EXCITATION

$$\mathbf{X^{+Z} + h\nu \rightleftharpoons X^{+Z*}}$$







- **Atomic quantities (constant numbers):**

- $\mathbf{A_{21}}$ for Spontaneous Decay or Radiative Decay Rate

- f (Oscillator Strength) or $\mathbf{B_{12}}$ for Excitation

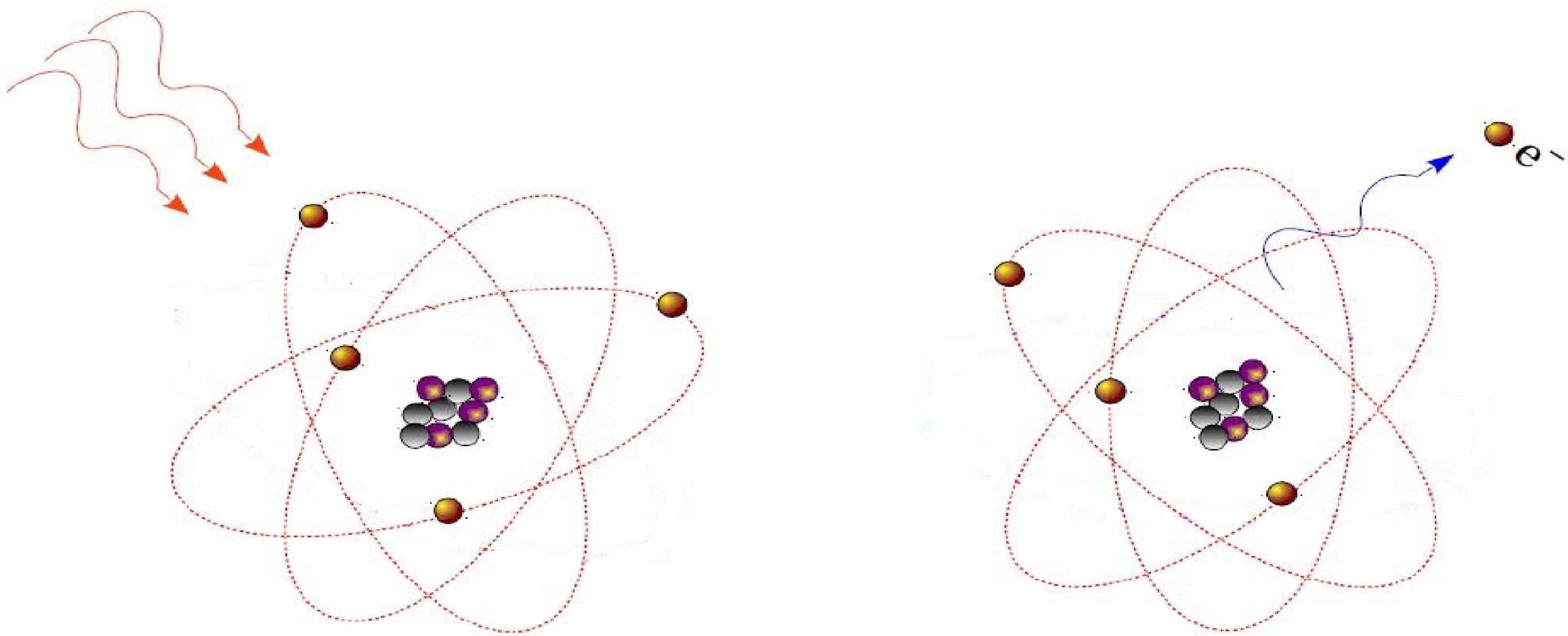
- **Monochromatic opacity (κ_ν) depends on $\mathbf{f_{ij}}$**

$$\kappa_\nu(\mathbf{i} \rightarrow \mathbf{j}) = \frac{\pi \mathbf{e^2}}{\mathbf{mc}} \mathbf{N_i f_{ij}} \phi_\nu$$

N_i = **ion density in state i,** ϕ_ν = **profile factor**

- κ **includes thousands to millions of transitions**

Opacity: PHOTOIONIZATION (PI):



i) Direct Photoionization (background):

$$\mathbf{X^{+Z} + h\nu \rightleftharpoons X^{+Z+1}} + \epsilon$$

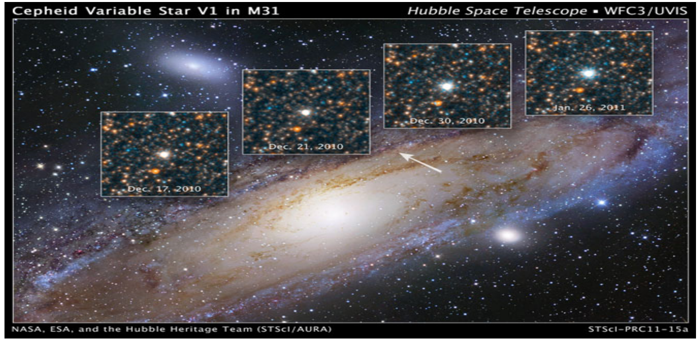
ii) Resonant Photoionization: an intermediate state before ionization → "Autoionizing state" → Resonant lines

$$\mathbf{X^{+Z} + h\nu \rightleftharpoons (X^{+Z})^{**} \rightleftharpoons X^{+Z+1}} + \epsilon$$

- κ_ν **depends on photoionization cross section** $\sigma_{\mathbf{PI}}$

$$\kappa_\nu = \mathbf{N_i}\sigma_{\mathbf{PI}}(\nu)$$

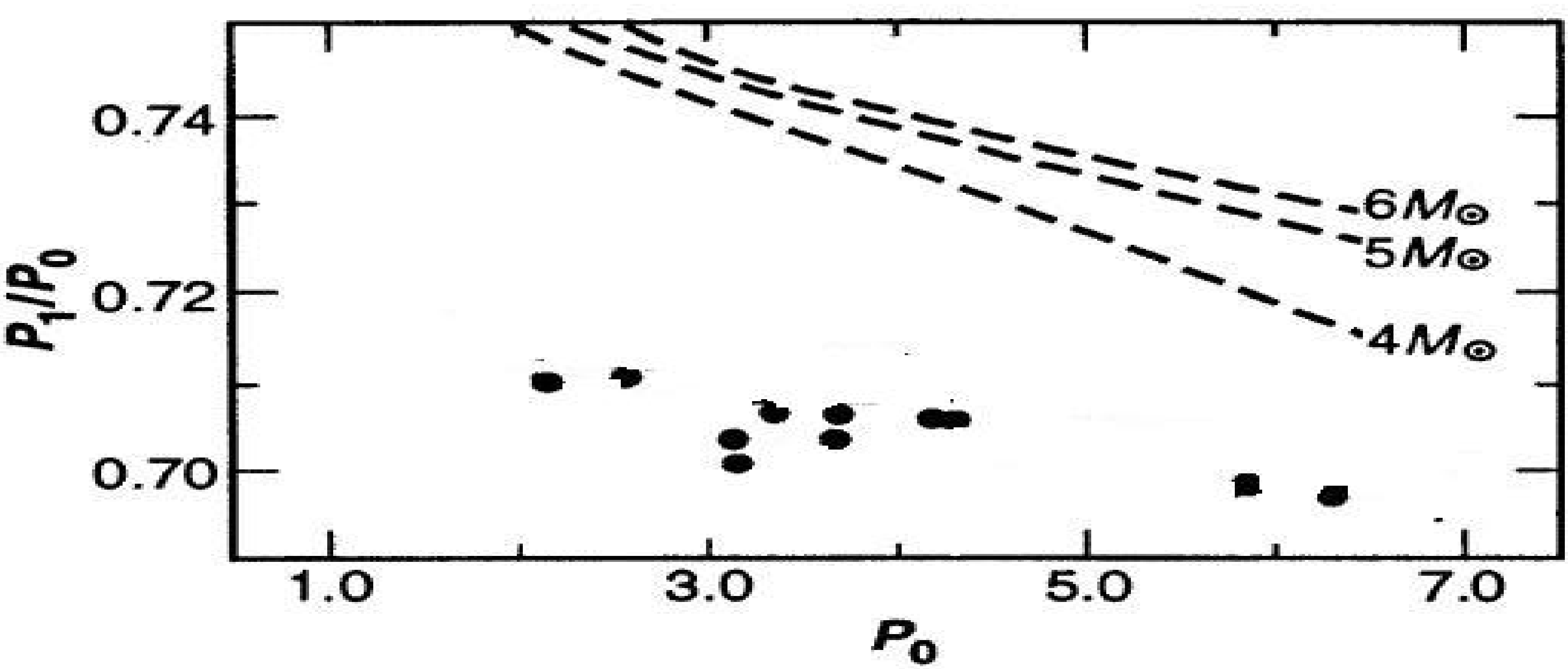
The OPACITY Project



The IRON Project

- Cepheid are stars, larger than the Sun, and go through periodic brightness and dimming states which can last for days to months
- Luminosity (M_v) is proportional to the mass and opacity

Discrepancy in predicted pulsation periods of Cepheid stars - REQUIRED HIGHER METALICITY/ OPACITY



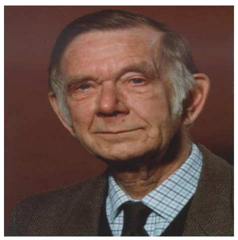
- Astronomers plea for accurate atomic physics to find more metalicity

The OPACITY Project (OP) & The IRON Project (IP)

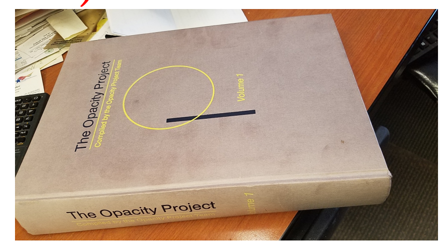
AIM: • Accurate Study of Atomic systems and process in astrophysical plasmas, • Obtain plasma opacities, • Applications to astrophysical problems

Needed: i) Development of Theory, ii) package of computer programs, and iii) a large team of scientists

•THE OPACITY PROJECT (OP) (1983 - 2007, 2007 -):



Prof. M.J. Seaton (1923 - 2007), UCL, UK



• The OP initiated and led by Seaton, - OP led to

• THE IRON PROJECT (IP) (1991 -)

CONTRIBUTORS: M.J. Seaton, W. Eissner, N. Badnell, M. Bautista, K.A. Berrington, AM Binello, P. Burke, V.M. Burke, K. Butler, G.X. Chen, MC Chidichimo, F. Delahaye, M Le Dourneuf, J.A. Fernley, M.E. Galavis, M Graziani, A. Hibbert, D.G. Hummer, A.E. Kingston, R Kisielius, D.J. Lennon, D. Luo, AE Lynas-Gray, H.E. Mason, M Melendez, C. Mendoza, D. Mihalas, M. Montenegro, S.N. Nahar, H. Nausbaumer, S Nakazaki, P. H. Norrington, P. Palmeri, G. Peach, J Pelan, A.K. Pradhan, P. Quinet, P Romano, H.P. Saraph, J.A. Tully, MC Witthoeft, Y. Yan, PR Young, C.J. Zeippen, V Zeman, G. Del Zenna, H.L. Zhang (52 authros)

OUTCOMES OF THE PROJECTS

New Physics:

- Solved many astrophysical problems
- Found new physics in photoionization - features & X-ray lines
- Unified method for electron-ion was introduced
- High precision radiative and collisional data for applications
- Found new applications in nanobiomedicine

Publications:

- The Opacity Project (TOP) series: 22 papers in JPB,
- The Iron Project (TIP) series: 68 in A&A + additional ones outside
- Book chapters, conference conference proceedings articles
- Book: The Opacity Project, The Opacity Project team, IOP (1995)
- Textbook: "Atomic Astrophysics and Spectroscopy" (A.K. Pradhan & S.N. Nahar, Cambridge University press, 2011)
- Atomic & Opacity Databases
- TOPbase (OP) at CDS: http://vizier.u-strasbg.fr/topbase/topbase.htm

- Energy levels, Oscillator Strengths, Photoionization Cross Sections

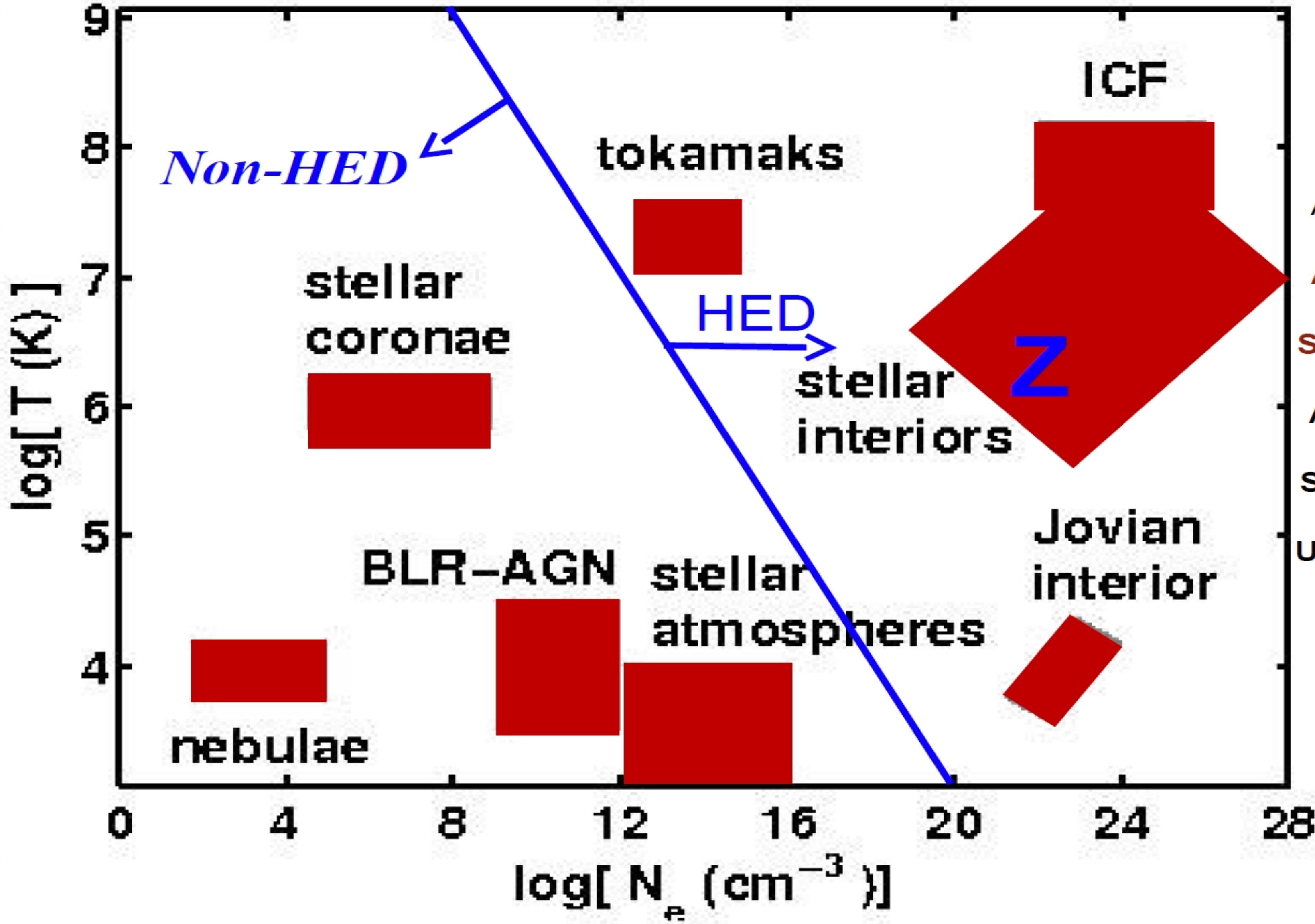
- TIPbase (IP) at CDS: http://cdsweb.u-strasbg.fr/tipbase/home.html

- Collisional Strengths for Electron Impact Excitations, and for Radiative Processes similar to TOPbase (not complete)

- OPserver for monochromatic opacities and program for mixtures at the OSC: http://opacities.osc.edu/
- NORAD-Atomic-Data at OSU: Latest radiative and electron-ion recombination data, http://norad.astronomy.ohio-state.edu

PLASMA COVERS 99% OF REGION IN T-ρ PHASE SPACE

Temperature-Density In HED Environments



Adapted From "Atomic Astrophysics And Spectroscopy"

Anil Pradhan and Sultana Nahar, (Cambridge University Press 2011)

- BLR-AGN (broad-line regions in active galactic nuclei), where many spectral features are associated with the central massive black hole
- Laboratory plasmas - tokamaks (magnetic confinement fusion devices), Z-pinch machines (inertial confinement fusion (ICF) devices)

Electron & Photon Distribution Functions in Plasmas

- The universe has largely charged particles and photons
- Temperature 'T' is defined differently for a radiation (photon) or the particle (electron)

$\mathbf{E = h\nu \sim kT}$, **or** $\mathbf{E = 1/2mv^2 = 3/2kT}$

- Example: Consider a star ionizing a molecular cloud into a gaseous nebula - These two objects, the star & the nebula, have different T distribution functions
- A plasma of charged particles and a radiation field of photons is treated with two distribution functions, Planck (for photons) and Maxwell (for electrons)

PLANCK DISTRIBUTION FUNCTION FOR PHOTONS

- Energy of the radiation emitted by a black body, e.g. a star, is described by the Planck distribution function

$$\mathbf{B_\nu(T_*) = \frac{2h\nu^3}{c^2}\frac{1}{\exp(h\nu/kT_*) - 1}}, \tag{1}$$

$T_* =$ ***radiation temperature***, $\nu =$ **frequency of the photons.**

• **Integrating $B_\nu(T_*)$ over the frequency, the radiance or energy per m^{2}sec emitted by an object at temperature T is given by Stefan-Boltzmann Law,**

$$\mathbf{E} = \sigma \mathbf{T}^{\mathbf{4}} \tag{2}$$

$\sigma = \mathbf{5.67} \times \mathbf{10^{-8}}$ **Watts/(m^2 K^4)= Stefan constant**

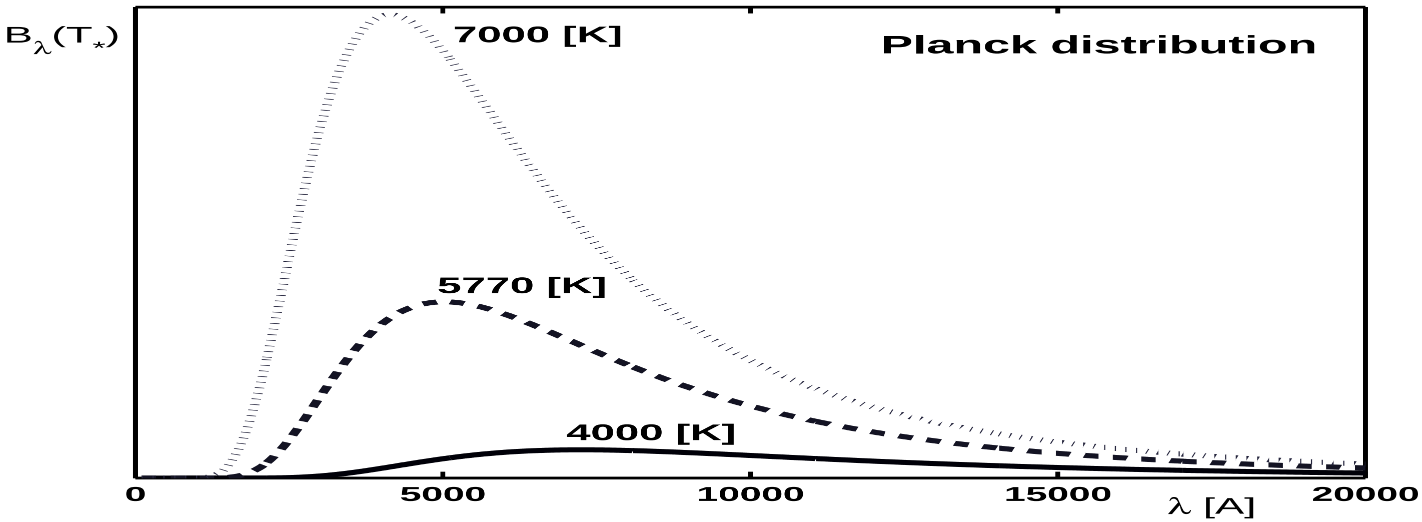
MAXWELL DISTRIBUTION FUNCTION FOR ELECTRONS

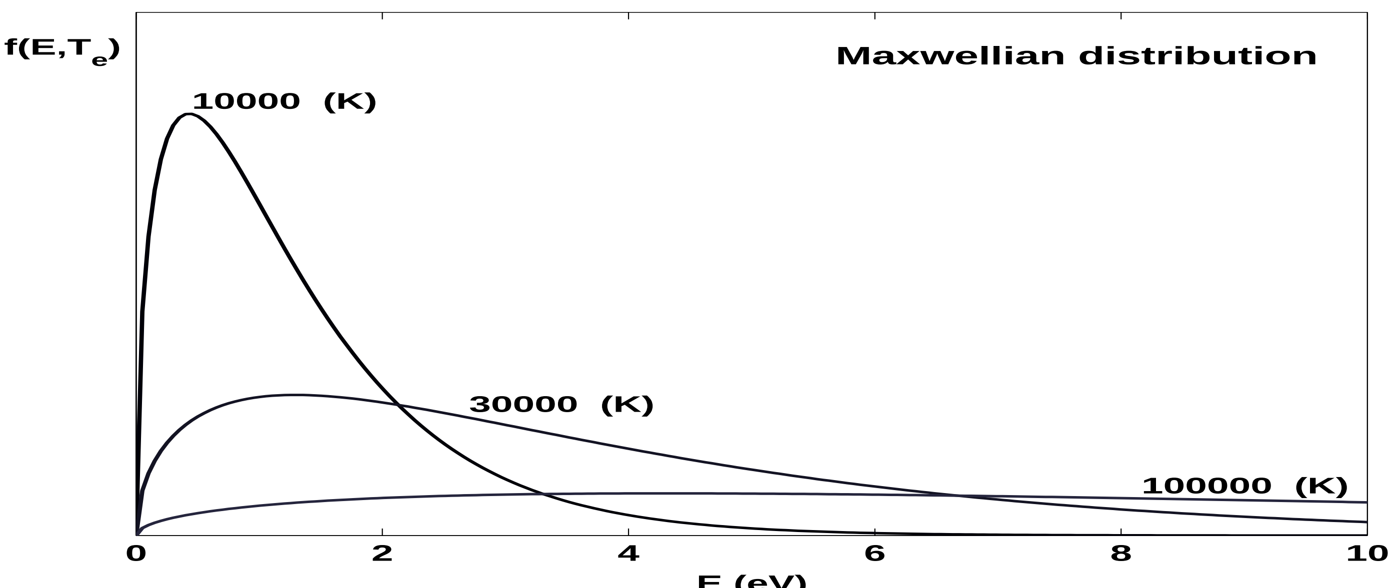
• **Energy or velocity of charged particles (electrons) in the plasma ionized or heated by a star, e.g. in an H∼II region at temperature T is described by the Maxwell distribution function**

$$\mathbf{f(v)} = \frac{\mathbf{4}}{\sqrt{\pi}}\left(\frac{\mathbf{m}}{\mathbf{2kT}}\right)^{\mathbf{3/2}} \mathbf{v^2 exp}\left(-\frac{\mathbf{mv^2}}{\mathbf{2kT}}\right). \tag{3}$$

• **Distribution functions describe the energy behaviors of the ensemble of photons and electrons. They are needed for astrophysical modelings, such as, computing the rate coefficients of the atomic processes.**

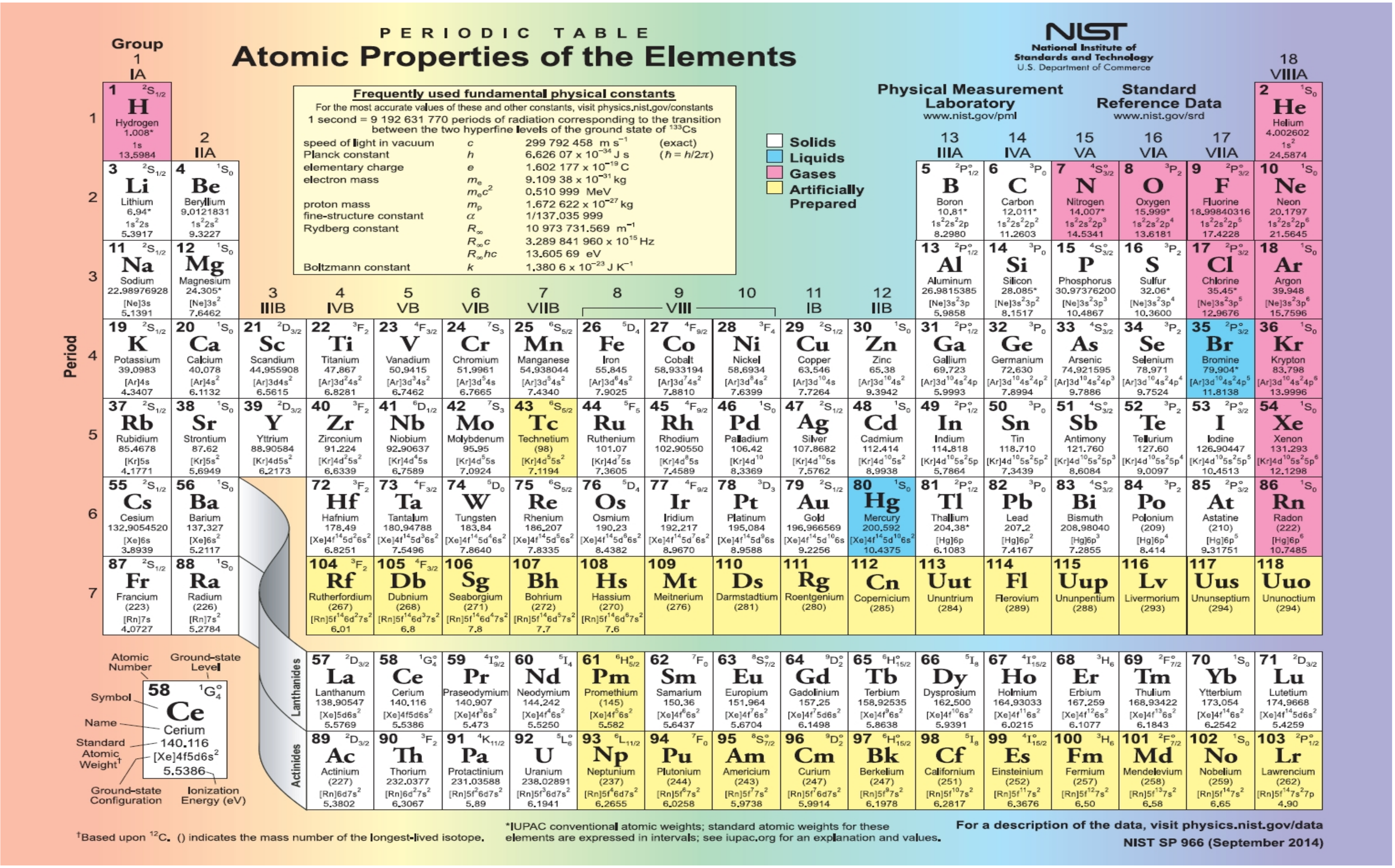
PLANCK & MAXWELL DISTRIBUTION FUNCTIONS





- TOP Fig: Solar surface $T_* = 5770\,\mathrm{K} \rightarrow$ peak black body emission - yellow ~5500 Å.
- Bottom Fig: H II region (nebula): Ionized by star black body radiation of $T \sim 30000$ - $40000\,\mathrm{K}$, electron KE of Maxwellian distribution - $\mathrm{T_e} \approx 10000 - 20000\,\mathrm{K}$

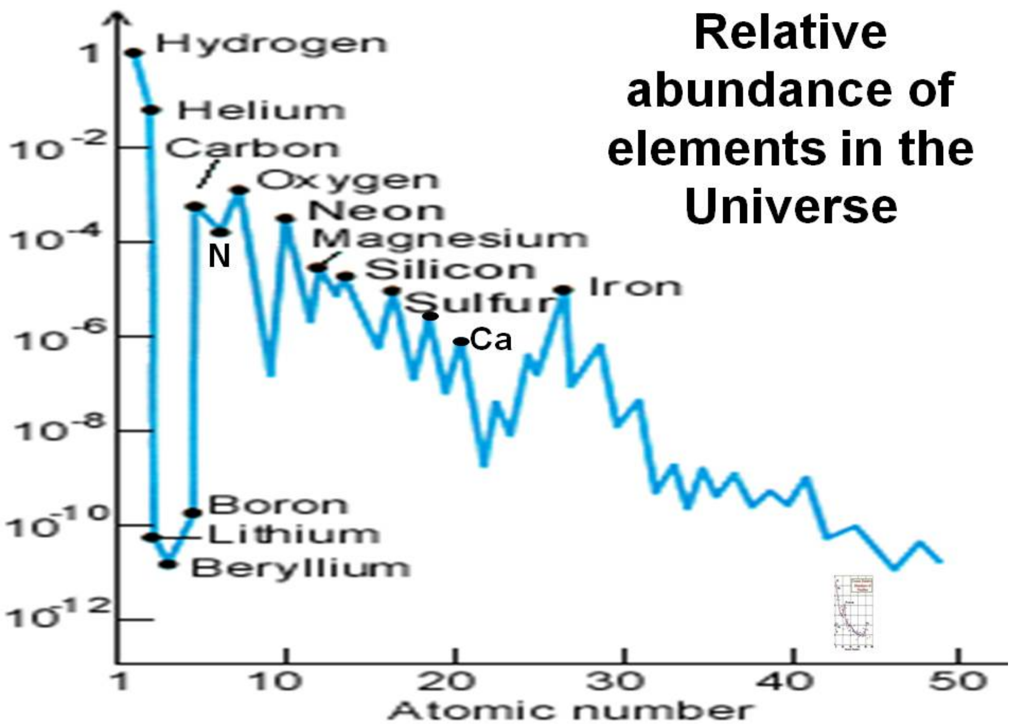
Atomic Structure: CONSTITUENTS OF MATTER CREATED BY STARS

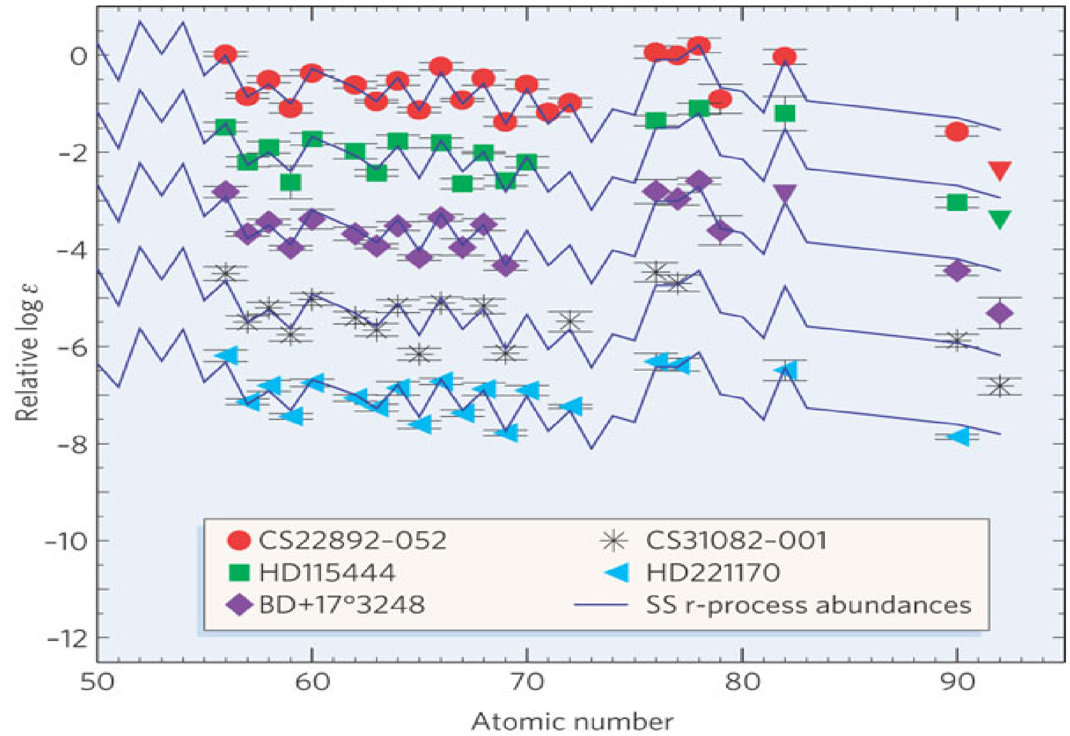


• Elements: Gases (pink), Solids (white), Liquids (blue). A lab generated yellow element is replaced with astrophysical observation

• Elements are created through nuclear fusion. It starts with creating He from 2 H atoms. As plasma density and T increase in the stellar core, Li, C, N, O etc are created, and the process continues up to Fe

ABUNDANCES OF HEAVY ELEMENTS IN SPACE





- Nuclear fusion cycle in a star ends at Fe (strongest nuclear force). Elemental abundances go down beyond Fe. Fortunate to have elemental abundances on the Earth. Solar system was made from debris of supernova explosions
- Heavy elements are created through neutron capture - s-process in the star and r-process during supernova explosions New! Kilonova - mergers of black holes and neutron stars
- Metals, only with 3%, provide the maximum information
- 99% of the matter exist in the plasma state

STUDYING ASTRONOMICAL OBJECTS

- 99% of known matter is plasma

ASTRONOMICAL objects are studied in three ways:

- **IMAGING:**

- Beautiful pictures of astronomical objects, Stars, Nebulae, Active Galactic Nuclei, Black hole Environments, etc

$\rightarrow$ Provides information of size and location of the objects

- **PHOTOMETRY:**

- Low resolution spectroscopy - Bands of Electromagnetic Colors ranging from X-ray to Radio waves

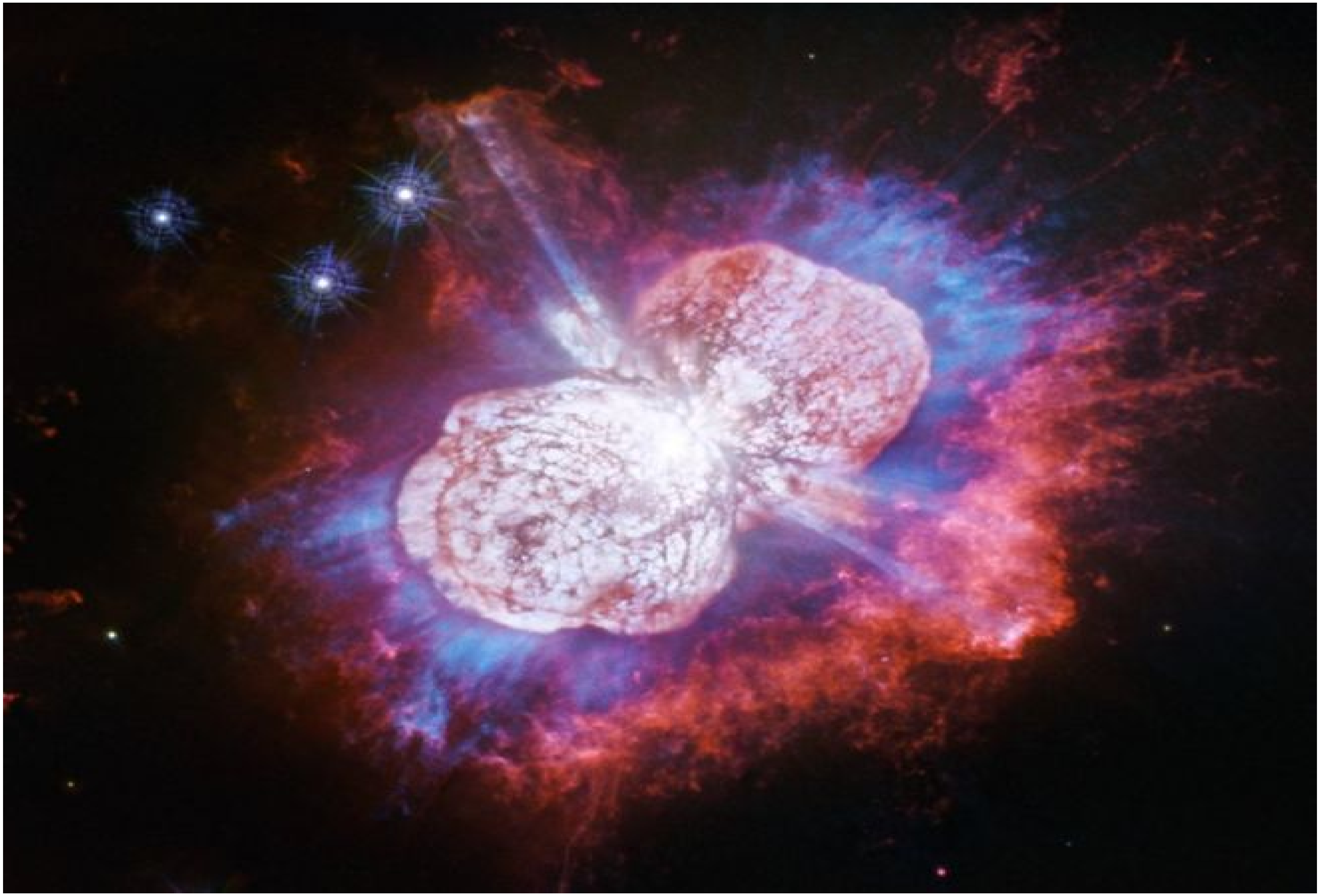
$\rightarrow$ macroscopic information

- **SPECTROSCOPY:**

- Taken by spectrometer - Provides most of the detailed knowledge: temperature, density, extent, chemical composition, etc. of astronomical objects

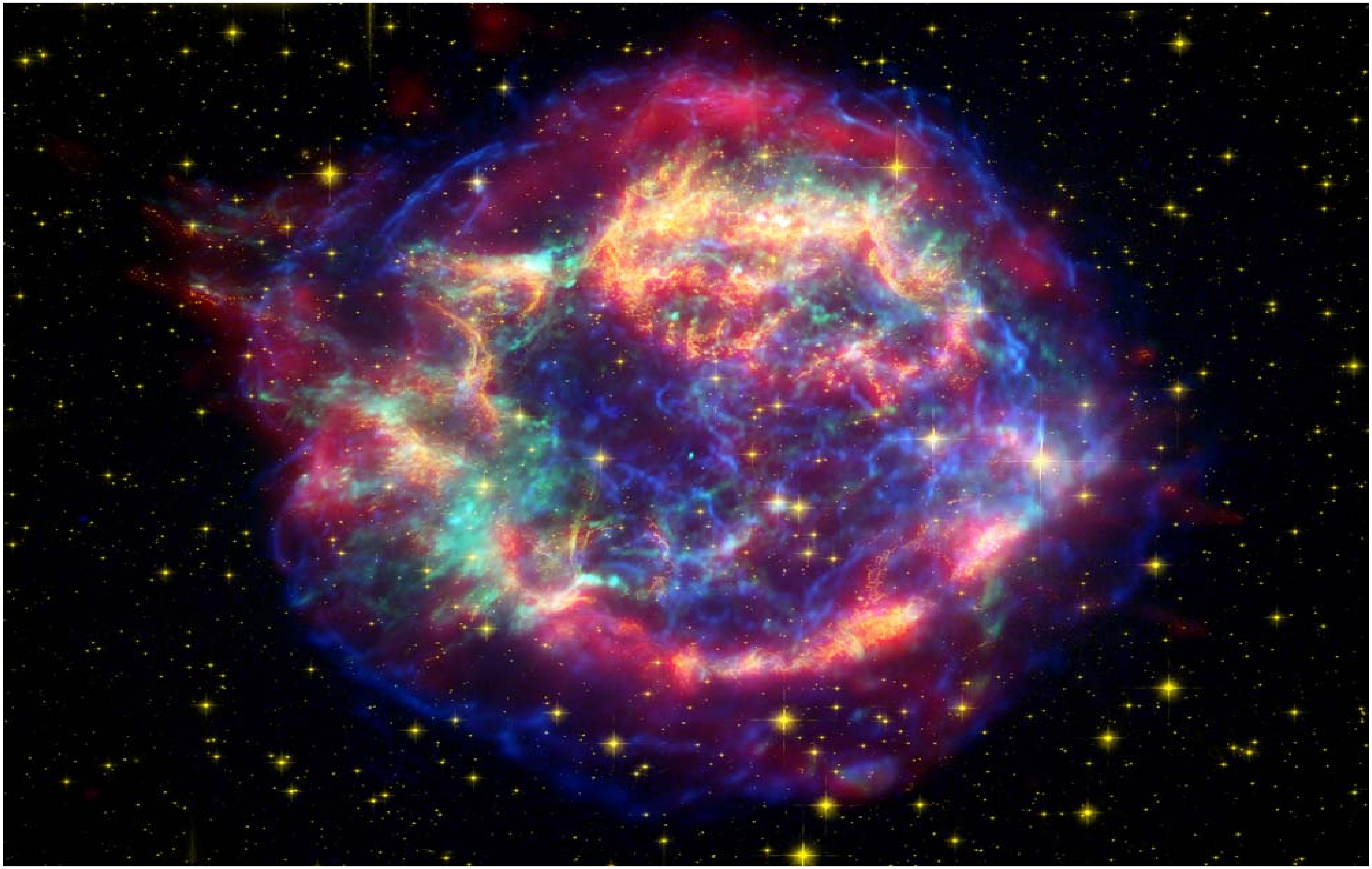
Spectroscopy is underpinned by Atomic & Molecular Physics

ETA CARINAE: IMAGE



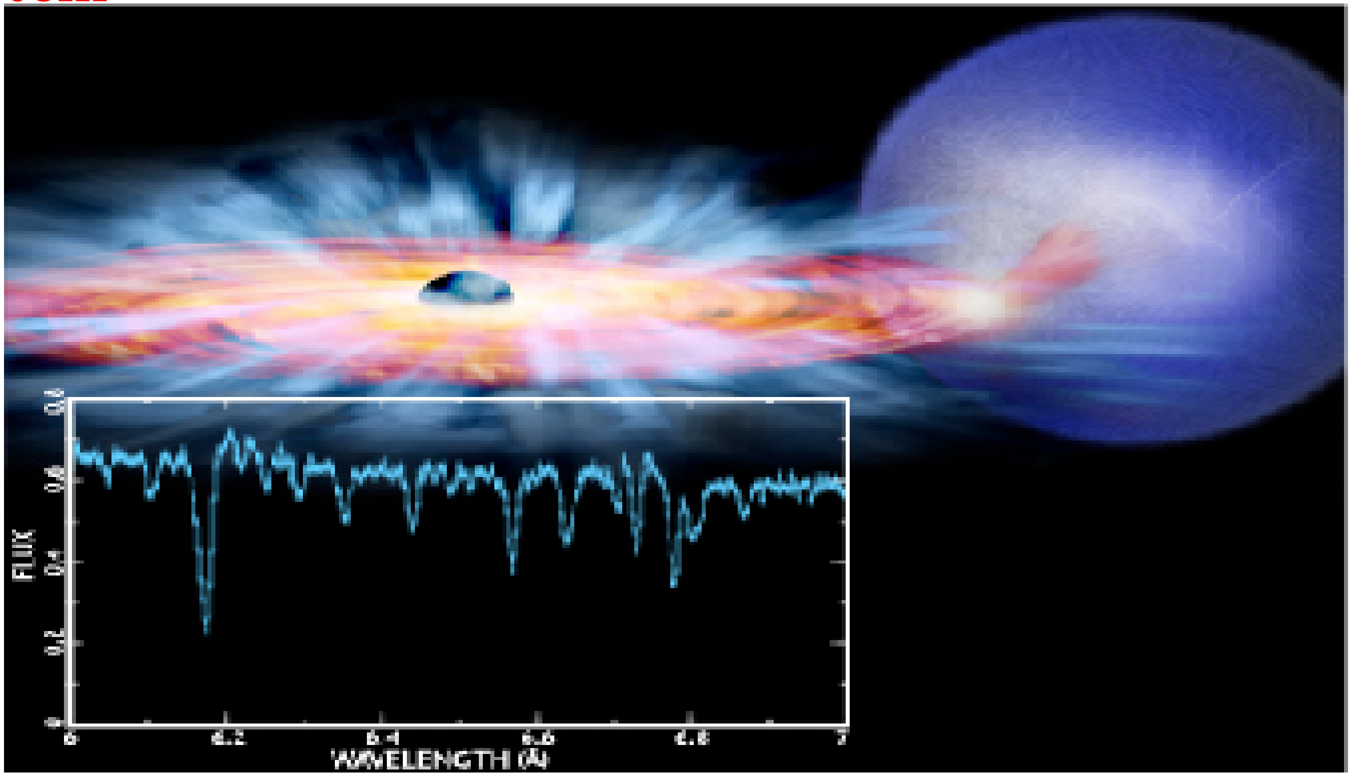
- Consists of 2 massive bright (5M times the sun) stars, heavier one went under a near supernova explosion
- Explosion produced two polar lobes, and a large but thin equatorial disk, all moving outward at 670 km/s. Mass indicates future eruptions
- HST image shows the bipolar Homunculus Nebula around it

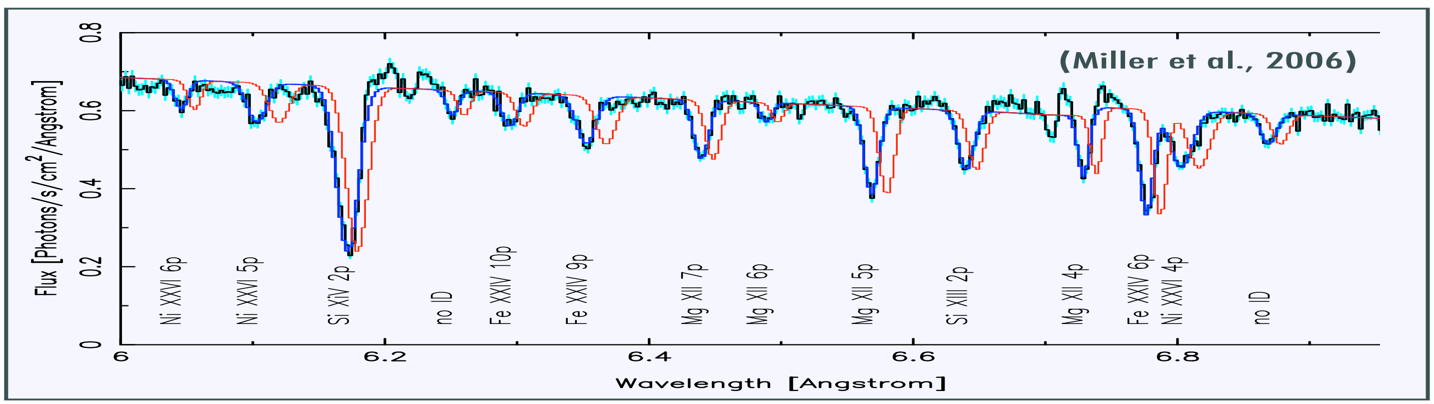
SUPERNOVA REMNANT CASSIOPEIA A: PHOTOMETRIC



- Photometric Observation: Spitzer (Infrared - red),
Hubble (Visible - yellow),
Chandra (X-ray - green & blue)
- Heavier elements - Supernova explosion
- Solar system made from debris of supernova explosions

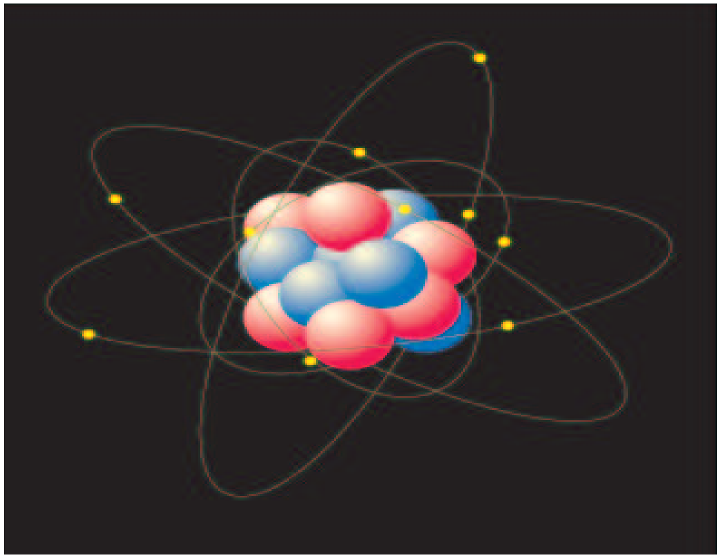
SPECTRUM of the Wind near Black hole: GRO J1655-40 Binary Star System

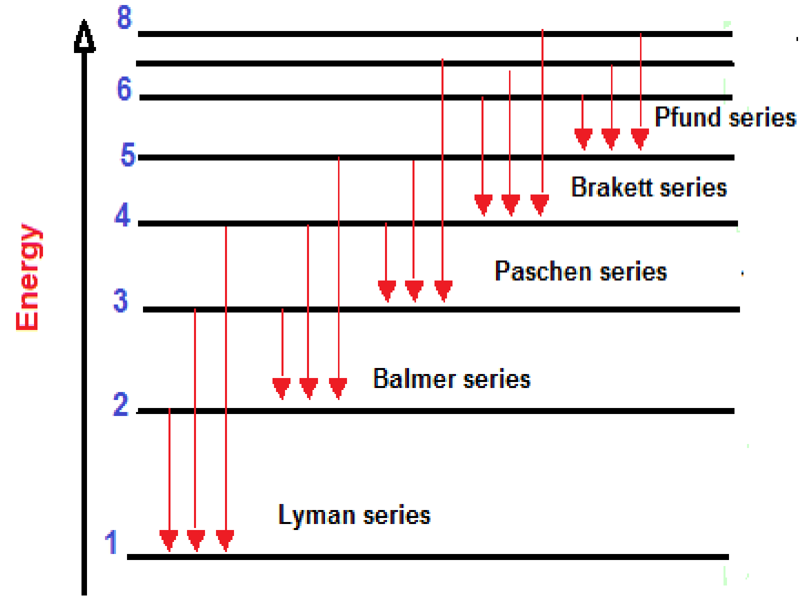


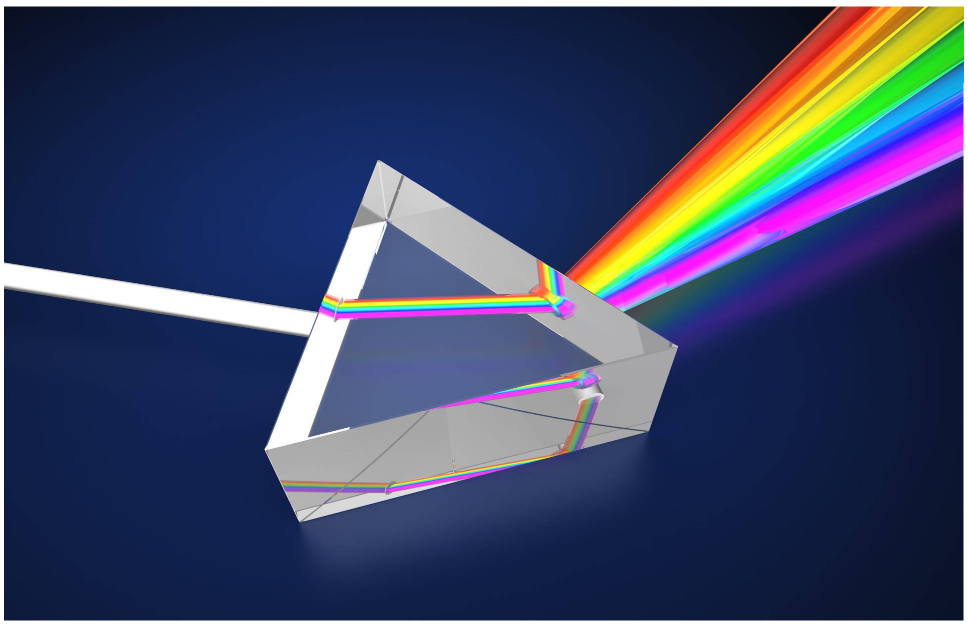


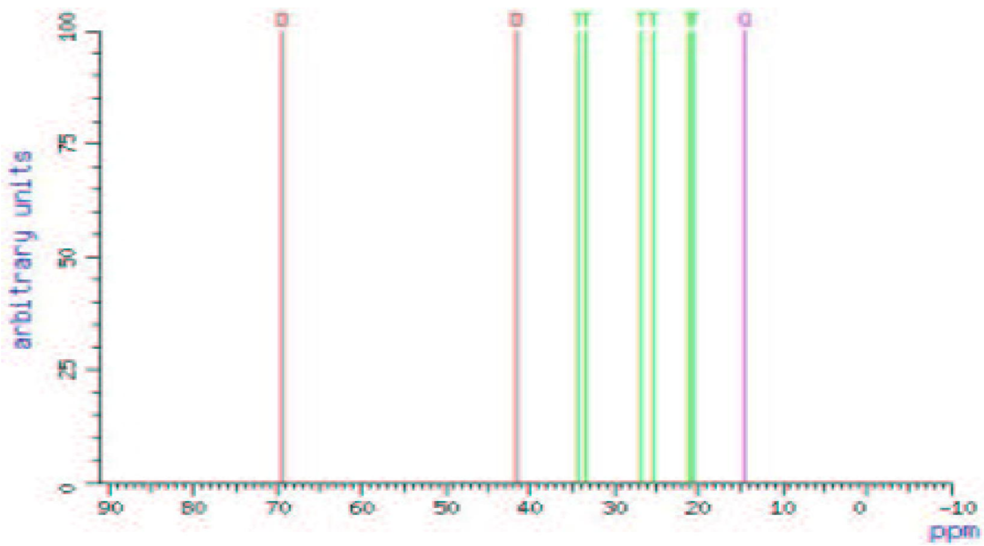
- Materials from the large star is sucked into companion black hole - form wind as they spiral to it. Spectrum of the wind (BLUE):
- Highly charged Mg, Si, Fe, Ni lines.RED: Elements in natural widths
- Doppler Blue Shift - Wind is blowing toward us

RADIATION FROM ATC









- Energy levels are quantized. There are infinite number of levels.
- An electron can be excited to higher levels. While dropping down, it gives out a photon. Radiation contains photons of many energies
- SPECTRUM: Splitting the radiation in to its colors: Rainbow, C
li

ATOMIC STRUCTURE

- **Atomic structure - i) Organization of electrons in various shells and subshells, ii) Determinations of electron energies and wave functions**
- **As Fermions, unlike Bosons, electrons form *structured* arrangements bound by the attractive nuclear potential**
- **Different atomic states arise from quantization of motion, orbital and spin angular momenta of all electrons. Transitions among those states involve photons which are seen as lines in observed spectra**
- **The combination of orbital angular momentum L and spin angular momentum S follow strict coupling rules, known as selection rules, that determine the stationary energy states and expectation values, such as, mean radius.**
- **The dynamic state of an atom - described by a Schrodinger equation**
- **HYDROGEN ATOM - only atomic system that can be treated exactly**
- **Approximation begins from 2-electrons systems**

HYDROGEN ATOM

Schrodinger equation of hydrogen, with KE = $\mathbf{P^2/(2m)}$ and nuclear potential energy $\mathbf{V(r)}$, is

$$\left[-\frac{\boldsymbol{\hbar}^{\mathbf{2}}}{\mathbf{2m}}\left(\nabla^{\mathbf{2}}\right) \quad + \quad V(r)\right]\Psi \;=\; E\;\Psi \tag{4}$$

$$or,\;\left[-\frac{\hbar^2}{2m}\left(\nabla_r^2+\nabla_\perp^2\right) \quad + \quad V(r)\right]\Psi \;=\; E\;\Psi$$

$$V(r) = -\frac{Ze^2}{r} = -\frac{2Z}{r/a_0}\,\mathrm{Ry}$$

In spherical coordinates

$$\nabla_{\mathbf{r}}^{\mathbf{2}} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) \tag{5}$$

$$\nabla_\perp^2 = \frac{1}{r^2\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right)+\frac{1}{r^2\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}$$

The solution or wavefunction has independent variables r, θ, ϕ, each will correspond to a quantum number,

$$\Psi(\mathbf{r},\vartheta,\varphi) \;=\; R(r)\;Y(\vartheta,\varphi)$$

ANGULAR EQUATION & m QUANTUM NUMBER

The angular equation is separated with constant λ as

$$\frac{\mathbf{1}}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial\mathbf{Y}}{\partial\vartheta}\right)+\frac{\mathbf{1}}{\sin^{\mathbf{2}}\vartheta}\frac{\partial^{\mathbf{2}}\mathbf{Y}}{\partial\phi^{\mathbf{2}}}+\lambda\mathbf{Y}=\mathbf{0} \tag{6}$$

The solutions are spherical harmonics,

$$\mathbf{Y}(\vartheta,\varphi)=\Theta(\vartheta)\ \Phi(\varphi) \tag{7}$$

The equation can be expressed in the form

$$\mathbf{L}^{\mathbf{2}}\mathbf{Y}(\vartheta,\varphi)=\left[-\frac{\hbar^{\mathbf{2}}}{\mathbf{2m}}\left(\nabla^{\mathbf{2}}\right)\right]\mathbf{Y}(\vartheta,\varphi)=\lambda\mathbf{Y}(\vartheta,\varphi), \tag{8}$$

L **is an angular momentum operator. Substituting** Y**,**

$$\frac{d^2\Phi}{d\varphi^2}+\nu\Phi=0, \tag{9}$$

$$\frac{1}{\sin\vartheta}\frac{d}{d\vartheta}\left(\sin\vartheta\frac{d\Theta}{d\vartheta}\right)+\left(\lambda-\frac{\nu}{\sin^2\vartheta}\right)\Theta=0\,,$$

where $\nu = m^2$**, and** $\Phi(\varphi) = (\mathbf{2}\pi)^{-\mathbf{1/2}}\ \mathrm{e}^{\mathbf{i m}\varphi}$**.** m **=*magnetic angular quantum number* and equals to** $0\,,\pm1,\ \pm2,\ldots$

ANGULAR EQUATION & l QUANTUM NUMBER

Replacing ϑ **by** $\mathbf{w} = \cos\vartheta$ **the** Θ **equation is**

$$\frac{d}{dw}\left[(1-w^2)\frac{d\Theta}{dw}\right] + \left[\lambda - \frac{m^2}{1-w^2}\right]\Theta(w) = 0. \tag{10}$$

A finite solution Θ **requires** $\lambda = \mathbf{l}(\mathbf{l}+\mathbf{1})$, **where** l **= 0, 1, 2... The solutions are associated Legendre polynomials of order** l **and** m**,**

$$\mathrm{P}_{\mathbf{l}}^{\mathbf{m}}(\mathbf{w}) = (\mathbf{1}-\mathbf{w}^{\mathbf{2}})^{|\mathbf{m}|/\mathbf{2}}\frac{\mathbf{d}^{|\mathbf{m}|}}{\mathbf{dw}^{|\mathbf{m}|}}\mathrm{P}_{\mathbf{l}}(\mathbf{w}), \tag{11}$$

$\mathbf{m} = \mathbf{l}, \mathbf{l}-\mathbf{1}, \ldots -\mathbf{l}$**.** $\mathbf{m} = \mathbf{0} \rightarrow \mathbf{P}_{l}(w)$ **= Legendre polynomial of order l. The angular solution of normalized spherical harmonic:**

$$\mathbf{Y}_{\mathbf{lm}}(\vartheta,\varphi) = \mathbf{N}_{\mathbf{lm}}\ \mathrm{P}_{\mathbf{l}}^{\mathbf{m}}(\cos\vartheta)\ \mathrm{e}^{\mathbf{im}\varphi} \tag{12}$$

where

$$\mathbf{N}_{\mathbf{lm}} = \epsilon\left[\frac{\mathbf{2l}+\mathbf{1}}{\mathbf{4}\pi}\ \frac{(\mathbf{l}-|\mathbf{m}|)!}{(\mathbf{l}+|\mathbf{m}|)!}\right]^{\mathbf{1}/\mathbf{2}}, \tag{13}$$

$\epsilon = (-1)^m$ **for** $m > 0$ **and** ϵ **= 1 for** $m \leq 0$**.**

ANGULAR MOMENTUM OPERATOR

Spherical harmonics satisfy the orthogonality condition

$$\int_{\varphi=0}^{2\pi}\int_{\vartheta=0}^{\pi} \mathbf{Y}^*_{\mathbf{l_1 m_1}}(\vartheta,\varphi)\mathbf{Y}_{\mathbf{l_2 m_2}}(\vartheta,\varphi)\ \mathbf{sin}\vartheta\,\mathbf{d}\vartheta\,\mathbf{d}\varphi = \delta_{\mathbf{l_1,l_2}}\ \delta_{\mathbf{m_1,m_2}} \tag{14}$$

The equation with angular momentum operator can now be written as

$$\mathbf{L^2 Y_l^m}(\vartheta,\varphi) = \mathbf{l(l+1)}\ \hbar^2\ \mathbf{Y_l^m}(\vartheta,\varphi) \tag{15}$$

With angular momentum $\mathbf{L = mvr = m\omega r^2}$ the angular frequency $\omega = \mathbf{L/mr^2}$, the centripetal force is $\mathbf{m\omega^2 r = L^2/mr^3}$ and the corresponding potential energy is

$$\mathbf{V_{ang}} = \frac{\mathbf{1}}{\mathbf{2}}\mathbf{m\omega^2 r^2} = \frac{\mathbf{L^2}}{\mathbf{2mr^2}}. \tag{16}$$

This is similar to the second potential term of hydrogen provided

$$\mathbf{L^2 = l(l+1)}\hbar^2\,; \tag{17}$$

THE RADIAL EQUATION

The radial equation representing the dynamical motion of the electron is

$$\left[\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)+\frac{2m}{\hbar^2}\Big(E-V(r)\Big)-\frac{\lambda}{r^2}\right]R(r)=0\,, \tag{18}$$

Substituting $R(r)=P(r)/r$, it is reduced to

$$\left[\frac{\hbar^2}{2m}\frac{d^2}{dr^2}-V(r)-\frac{l(l+1)\hbar^2}{2mr^2}+E\right]P(r)=0\,. \tag{19}$$

The equation shows motion of a particle in a potential

$$V(r)+\frac{l(l+1)\hbar^2}{2mr^2}\,, \tag{20}$$

We switch to Rydberg unit for the Schrodinger equation,

$$\left[\frac{d^2}{d(r/a_0)^2}+\frac{2Z}{r/a_0}-\frac{l(l+1)}{(r/a_0)^2}+E/\mathrm{Ry}\right]P(r)=0 \tag{21}$$

$$\text{or,}\quad\left[\frac{d^2}{dr^2}-V(r)-\frac{l(l+1)}{r^2}+E\right]P(r)=0\,, \tag{22}$$

SOLVING RADIAL EQUATION

- **The radial equation can be solved on specifying boundary conditions, (i) r at ∞, and (ii) r near $r = 0$**
- **The bound electron moves in the nuclear attractive potential: $\lim_{r\to\infty} V(r) = 0$. Hence for case (i) for $r \to \infty$**

$$\left[\frac{\mathbf{d^2}}{\mathbf{dr^2}} + \mathbf{E}\right] \mathbf{P}(\mathbf{r}) = \mathbf{0}\,, \tag{23}$$

which has solutions

$$\mathbf{P}(\mathbf{r}) = \mathrm{e}^{\pm\mathbf{ar}}, \qquad \mathbf{a} = \sqrt{-\mathbf{E}}\,. \tag{24}$$

Taking $E < 0$ for bound states, $\lim_{\mathbf{r}\to\infty} \mathrm{e}^{-\mathbf{ar}}$ is a possible solution. It is also valid for $E > 0$, when a becomes imaginary. Hence, the asymptotic behavior suggests

$$\mathbf{P}(\mathbf{r}) = \mathrm{e}^{-\mathbf{ar}}\mathbf{f}(\mathbf{r}) \tag{25}$$

subject to $\lim_{\mathbf{r}\to\mathbf{0}} \mathbf{f}(\mathbf{r}) = \mathbf{0}$. On substitution,

$$\frac{\mathbf{d^2f}}{\mathbf{dr^2}} - \mathbf{2a}\frac{\mathbf{df}}{\mathbf{dr}} + \left[\frac{\mathbf{2Z}}{\mathbf{r}} - \frac{\mathbf{l(l+1)}}{\mathbf{r^2}}\right] \mathbf{f}(\mathbf{r}) = \mathbf{0} \tag{26}$$

WAVEFUNCTION & n QUANTUM NUMBER

- For $r << 1$, the solution $f(r)$ is expressed as a power series

$$f(r) = r^s[A_0 + A_1 r + A_2 r^2 + \ \ldots \ ]$$

Finite f as $r \to 0$ requires $s > 0$ for consistent behavior of a bound electron. The possible radial wave function is

$$P(r) = f(r)e^{-ar} \approx r^{l+1}e^{-ar} \tag{27}$$

at large distances r. This again diverges at infinity, unless the series for f terminates at a point where the energy is

$$E = -(Z^2/n^2) \times \mathrm{Ry}\,; \tag{28}$$

n is a positive integer & defined as the *principal quantum number*. Full P(r) in Laguerre polynomial L is,

$$P_{nl}(r) = \sqrt{\frac{(n-l-1)!Z}{n^2[(n+l)!]^3 a_0}} \left[\frac{2Zr}{na_0}\right]^{l+1} e^{\frac{-Zr}{na_0}} \times L\,{}^{2l+1}_{n+l}\left(\frac{2Zr}{na_0}\right),$$

where

$$L^{2l+1}_{n+l}(\rho) = \sum_{k=0}^{n-l-1} \frac{(-1)^{k+2l+1}[(n+l)!]^2\rho^k}{(n-l-1-k)!(2l+1+k)!k!}\,. \tag{29}$$

QUANTUM DESIGNATION OF A STATE

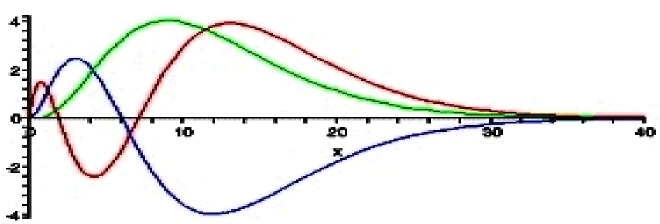
- **Atomic Shells: n = 1,2,3,4 .. = K,L,M,N**

- No of electrons = $2n^2$ - Closed shell, $< 2n^2$ - Open Shell

- **Orbital angular momentum: l=0,1,2,3,4...(n-1) = s,p,d,f,.**
- **Total Angular Momentum: L=0,1,2,3,4, ... , = S,P,D,F,..**
- **Magnetic angular momentum: $m_l = 0,\pm1,\pm2,\pm3,4 ..\pm l$**

(2l+1) values $\rightarrow$ angular momentum multiplicity = 2L+1

- **Spin angular momentum S was introduced due to electron spin. It is inherent in Dirac equation. S = integer or 1/2 integer depending on number of electrons with spin s=1/2**
- **Spin magnetic angular momentum = $m_s = \pm S$ - (2S+1) values - spin multiplicity**
- **Spin multiplicity = 1,2,3, .. =singlet, doublet, triplet ..**
- **Total angular momentum: $J = |L \pm S|$, $J_M = 0,\pm1,\pm2,\pm3,4 ..\pm J$, J multiplicity = $2J + 1$**
- **Parity (introduced from wavefunction) = π = $(-1)^l$ = +1 (even) or -1 (odd)**
- **Symmetry of a state: $^{(2S+1)}L^{\pi}$ (LS), $^{(2S+1)}L^{\pi}_{J}$ (LSJ - fine structure)**
- **No of nodes in a wavefunction= n-l-1**



SPECTRAL LINES & RYDBERG FORMULA

Hydrogen spectral line - Photon emitted or absorbed is of energy (Rydberg formula)

$$\boldsymbol{\Delta}\mathcal{E}_{\mathbf{n},\mathbf{n}'} = \frac{\mathbf{1}}{\lambda} = \mathcal{R}_{\mathrm{H}}\left[\frac{\mathbf{1}}{\mathbf{n}^{\mathbf{2}}} - \frac{\mathbf{1}}{\mathbf{n}'^{\mathbf{2}}}\right] \quad (\mathbf{n}' > \mathbf{n}), \tag{30}$$

where $\mathcal{R}_{\mathrm{H}} = \mathbf{109,677.576}\,/\mathrm{cm} = \mathbf{1/911.76}\,/\text{Å}$ **is the Rydberg constant. Energy in wavelength in Ångström units:**

$$\lambda = \frac{\mathbf{911.76}\,\text{Å}}{\boldsymbol{\Delta}\mathbf{E}/\mathrm{Ry}}. \tag{31}$$

- $\Delta\mathcal{E}_{n,n'}$ **yields series of spectral lines,**

$\mathcal{R}_{\mathrm{H}}\left[1 - \frac{1}{n'^2}\right],\ n' = 2, 3, 4, \ldots$ **Lyman (Ly)**

$\mathcal{R}_{\mathrm{H}}\left[\frac{1}{2^2} - \frac{1}{n'^2}\right],\ n' = 3, 4, 5, \ldots$ **Balmer (Ba)**

$\mathcal{R}_{\mathrm{H}}\left[\frac{1}{3^2} - \frac{1}{n'^2}\right],\ n' = 4, 5, 6, \ldots$ **Paschen (Pa)**

$\mathcal{R}_{\mathrm{H}}\left[\frac{1}{4^2} - \frac{1}{n'^2}\right],\ n' = 5, 6, 7, \ldots$ **Brackett (Br)**

$\mathcal{R}_{\mathrm{H}}\left[\frac{1}{5^2} - \frac{1}{n'^2}\right],\ n' = 6, 7, 8, \ldots$ **Pfund (Pf)**