UNIVERSITY OF ZAGREB

Faculty of Electrical Engineering and Computing

FunTomP

Functionalized Tomato Products

Machine learning and spectroscopy

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PRIMA

PARTNERSHIP FOR RESEARCH AND INNOVATION IN THE MEDITERRANEAN AREA

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https://itsoftware.com.co/content/structured-vs-unstructured-data/

Data – Information - Knowledge

John Naisbitt (1982) wrote: **"We are drowning in information but starved for knowledge".**

The data is raw, it simply exists and has no other meaning and meaning than its existence.

Information is data that is given meaning through a relational connection.

Knowledge is a suitable collection of information and such that it can be considered useful.

Knowledge are patterns in data or models which explain them.

Machine learning

https://www.udacity.com/course/machine-learning--ud262

Machine learning must be one of the fastest growing fields in computer science.

It is not only that the data is continuously getting “bigger,” but also the theory to process it and turn it into knowledge.

In various fields of science, from astronomy, physics, chemistry to biology, but also in everyday life, as digital technology increasingly infiltrates our daily existence, as our digital footprint deepens, more data is continuously generated and collected.

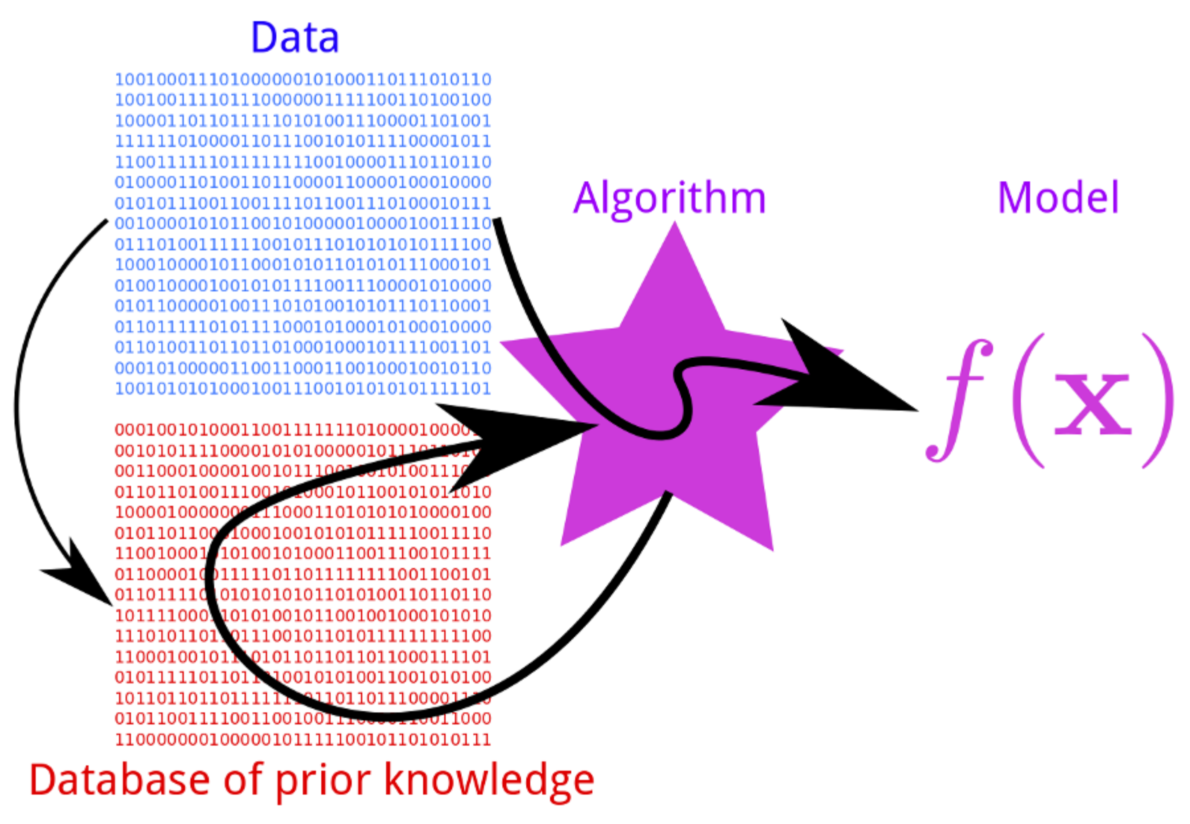
Machine learning

https://www.udacity.com/course/machine-learning--ud262

Whether scientific or personal, data that just lies dormant passively is not of any use, and smart people have been finding ever new ways to make use of that data and turn it into a useful product or service.

In this transformation, **machine learning** plays a larger and larger role.

Machine learning

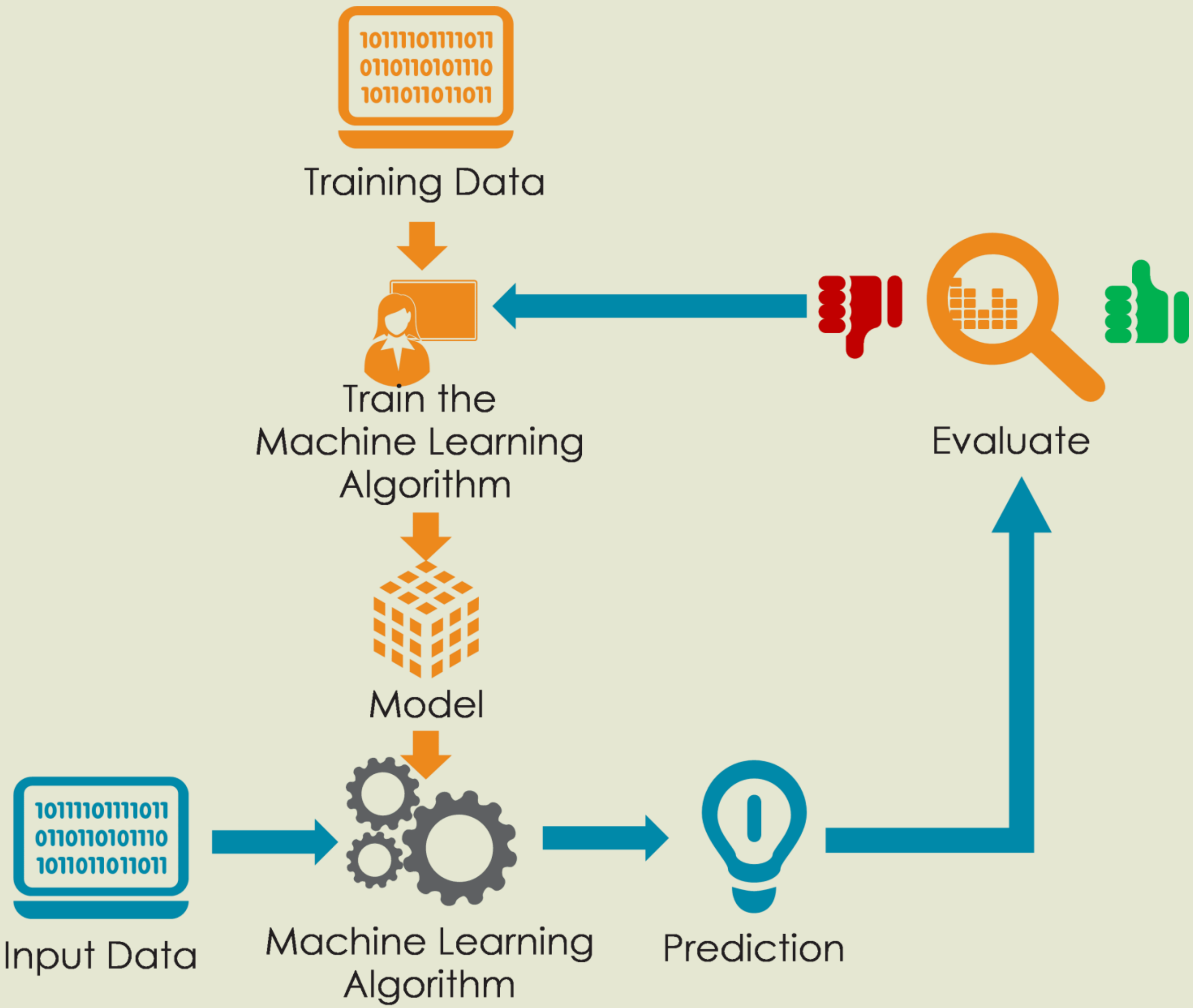


https://medium.com/@kaykwaalk/difference-between-an-algorithm-and-a-model-in-machine-learning-5d6b7297cce9

The **machine learning process** begins with **observations of data**, such as examples, direct experience or instruction.

ML looks for **rules, patterns or models in data** so it can later make inferences based on the examples provided.

The primary aim of ML is **to allow computers to learn autonomously without human intervention or assistance and adjust actions accordingly.**



https://intellipaat.com/blog/tutorial/data-science-tutorial/modeling-the-data/

Machine learning

ML has proven valuable because **it can solve problems at a speed and scale that cannot be duplicated by the human mind alone**.

With massive amounts of computational ability behind a single task or multiple specific tasks, machines can be trained **to identify patterns in and relationships between input data** and **automate routine processes**.

Machine learning: Data is key

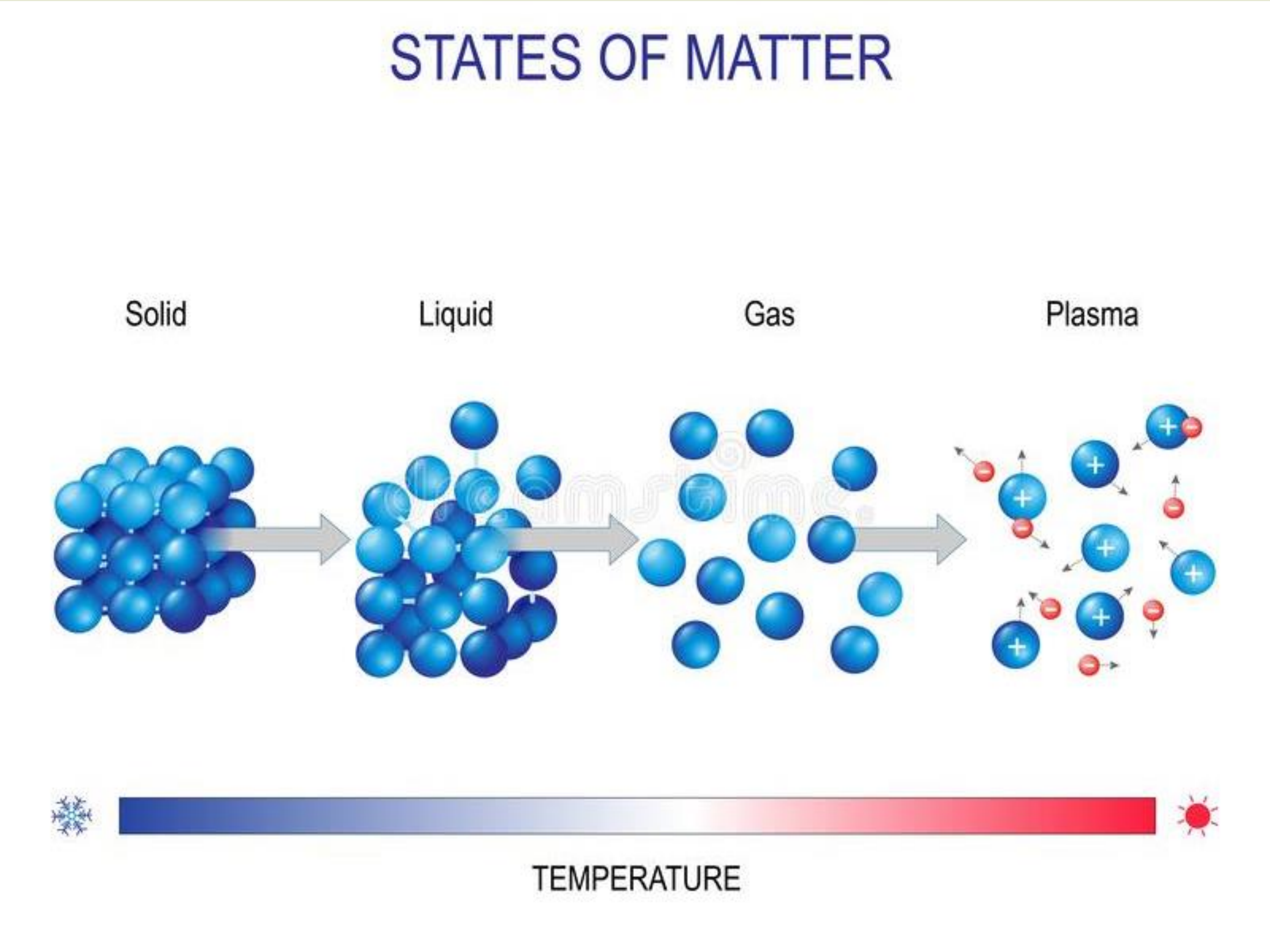
https://www.businessprocessincubator.com/content/safeguarding-data-ensuring-privacy/

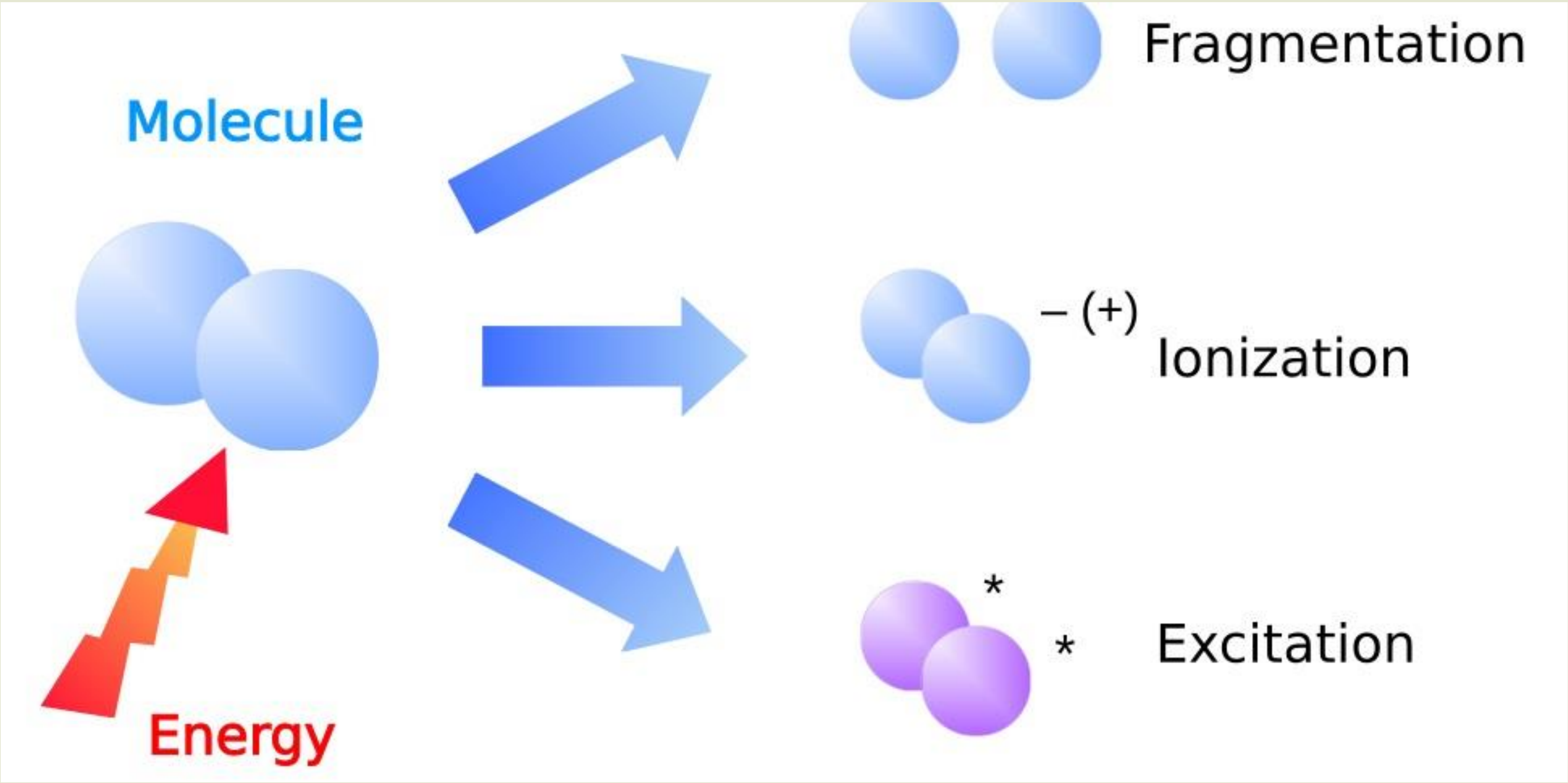
The **algorithms** that drive machine learning are critical to success.

ML algorithms build a mathematical model-based sample data, known as **"training data" to make predictions or decisions** without being explicitly programmed to do so.

This can reveal trends within data that information businesses can use **to improve decision making, optimize efficiency and capture actionable data at scale**.

The goal of ML: **<u>to build models that generalize well.</u>**


STATES OF MATTER
Solid
Liquid
Gas
Plasma
TEMPERATURE


Molecule
Energy
Fragmentation
– (+)
Ionization
*
*
Excitation

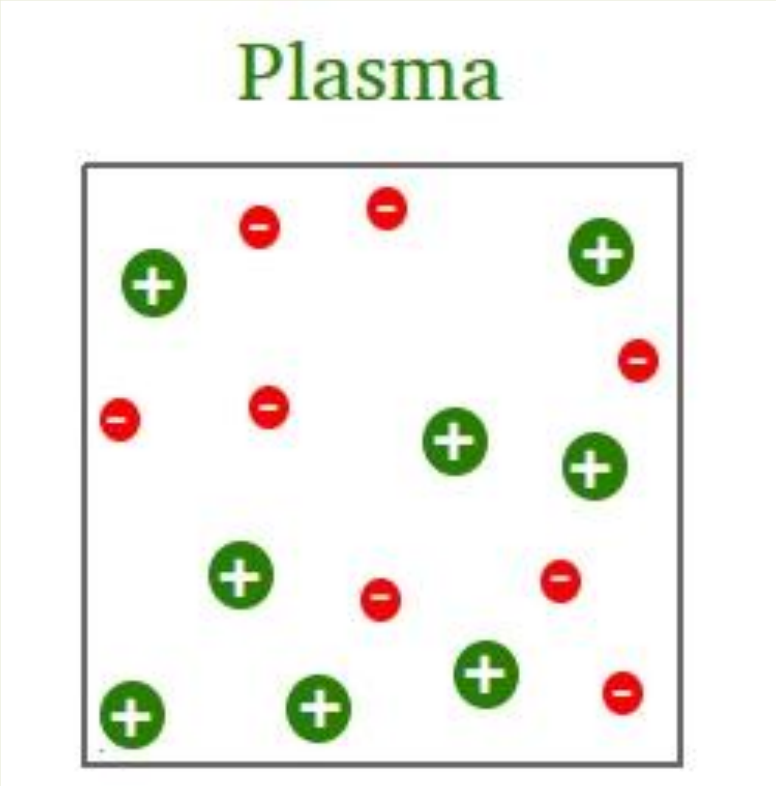
Plasma – state of matter

Plasma, in physics, an electrically conducting medium in which there are roughly equal numbers of positively and negatively charged particles, produced when the atoms in a gas become ionized.

It is sometimes referred to as **the fourth state of matter**, distinct from the solid, liquid and gas states.

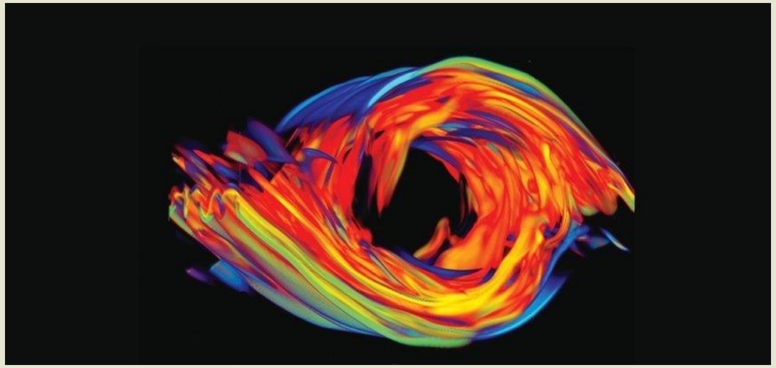
The negative charge is usually carried by **electrons**.

The positive charge is typically carried by atoms or molecules that are missing those same electrons, they are **ions**.



https://www.britannica.com/science/plasma-state-of-matter

Plasma – state of matter

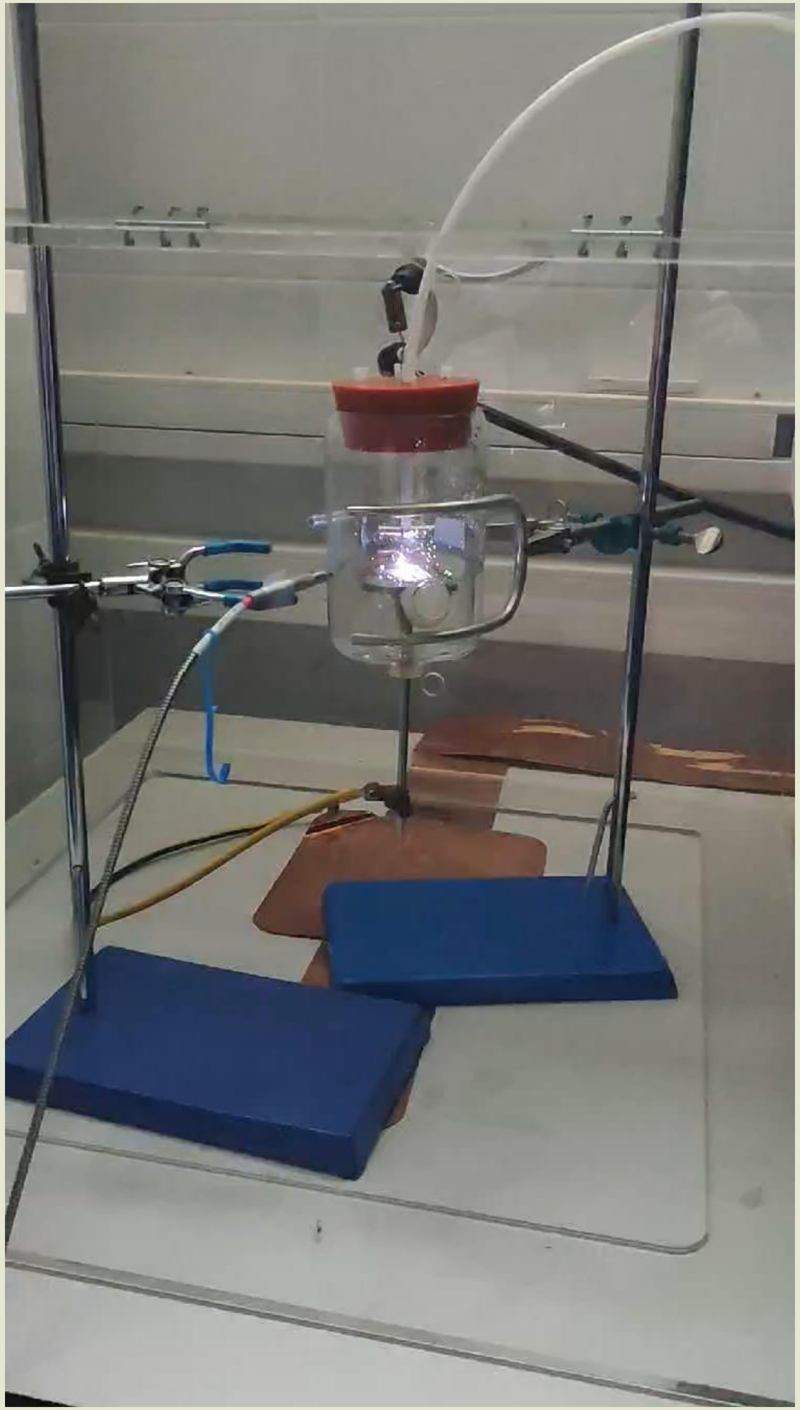


In some cases, **electrons** missing from one type of atom or molecule become attached to another component, resulting in a plasma containing both positive and negative **ions**.

The uniqueness of the plasma state is due to the importance of **electric and magnetic forces** that act on a plasma in addition to such forces as gravity that affect all forms of matter.

Since these electromagnetic forces can act at large distances, a plasma will act collectively much like a **fluid** even when the particles seldom collide with one another (**magnetohydrodynamical description of plasma fluid - MHD**).

https://www.britannica.com/science/plasma-state-of-matter



The **experimental set-up** consisted of a glass reactor (300-1000 mL) with a point-to-plate electrode configuration.

A medical stainless-steel needle was used as a HV electrode and stainless-steel electrode was a ground electrode.

Plasma was generated in liquid and gas phase through the capacitor charged with the pulsed HV power supply (IMPEL HVG60/1) to create electrical discharges up to maximal 50 kV; frequency range was 0-300 Hz.

Plasma diagnostics was done with Ocean FX extended range model (OCEAN-FX-XR1-ES) of **optical emission spectrometer** (OES).

The emission of a certain volume in the plasma chamber was delivered by an optical fiber to the spectrometer.

Optical emission spectrometer (OES)

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OCEAN-FX-XR1-ES	**Ocean FX extended-range model spectrometer preconfigured for 200-1025 nm wavelength range, with 25 Âµm slit and lens for enhanced sensitivity**
P600-2-SR	600 um Fiber, solarization-resistant, 2 m
74-UV	UV/VIS Collimating Lens, 200-2500 nm
OCEANVIEW	OceanView spectroscopy software with graphical user interface; accessible by download only from our secure server

OPTICAL EMISSION SPECTROSCOPY (OES) FOR PLASMA ANALYSIS

Plasma composition is a critical parameter in all types of plasma applications.

"Optical emission spectroscopy" is a common term for techniques that measure **optical absorption/emission spectra**, i.e., the light being emitted when a sample is being excited.

OES is an important technique in plasma analysis, where it enables **accurate non-contact characterization** of the color of the plasma and thus the species present.

Crucially, **OES is compatible with thermal and non-thermal plasma environments and applications** that are sensitive to contamination because it is the ideal **non-invasive measurement technique for plasma diagnostics** in hostile plasma environments while **preventing contamination**.

Additionally, OES provides **near-real-time feedback**.

OPTICAL EMISSION SPECTROSCOPY (OES) FOR PLASMA ANALYSIS

However, plasmas are typically characterized by a **large number of closely-spaced emission peaks.**

Separating these peaks requires an OES system with **high spectral resolution**.

Previous research on OES measurements of plasma processes has largely focused on plasma monitoring, species identification, and determination of the **electron temperature T_e and electron density n_e**.

In order to use the OES method to determine these parameters, one usually applies the so-called **line intensity ratio method**, which requires **a relative intensity calibrate spectroscopic system** and **a suitable physics-based model for excited species in the plasmas to be investigated.**

https://pearl.kaeri.re.kr/pearl/crmodel/lineratio.jsp

Line Intensity Ratio

In optical plasma diagnostics, line intensity ratio method is one of method to determine electron temperature and density of plasma. The intensity of radiation, I_{ki}, is expressed by

$$I_{ki} = E(k,i)_{ki} N_k A_{ki}$$

E_{ki} : Difference between energy levels E_k and E_i ($E_k > E_i$)
A_{ki} : Transition probability
N_k : Population of upper energy state of k.

Line intensity ratio of plasma is expressed by

$$\mathbb{L} = \frac{I_{ki}}{I_{pq}} = \frac{\lambda_{pq} N_k A_{ki}}{\lambda_{ki} N_p A_{pq}}$$

λ_{ki} : Wavelength corresponding to the transition from energy state k to energy state i.

In experiment, the optical system cannot collect whole radiation from plasma volume, the transmittance of optical system has a dependency on wavelength, and quantum efficiency of detecting system is also dependent on a wavelength. Thus, the measured line intensity ratio needs to be relatively calibrated for whole optical system and detector.

Boltzmann plot

The spectroscopic data also was used for estimating the temperature of the produced plasma and it is carried out using **Boltzmann plot**:

$$\ln\left(\frac{I}{\lambda g A}\right) = -\frac{1}{k_B T}E + \ln\left(\frac{4\pi Z}{hcn_0}\right)$$

I is intensity of the spectral line,

λ is wavelength of spectral line,

g is statistical weight of the energy level,

A is transition probability,

k_B is Boltzmann constant,

T is temperature,

E is energy level of the upper state for emission,

Z is partition function,

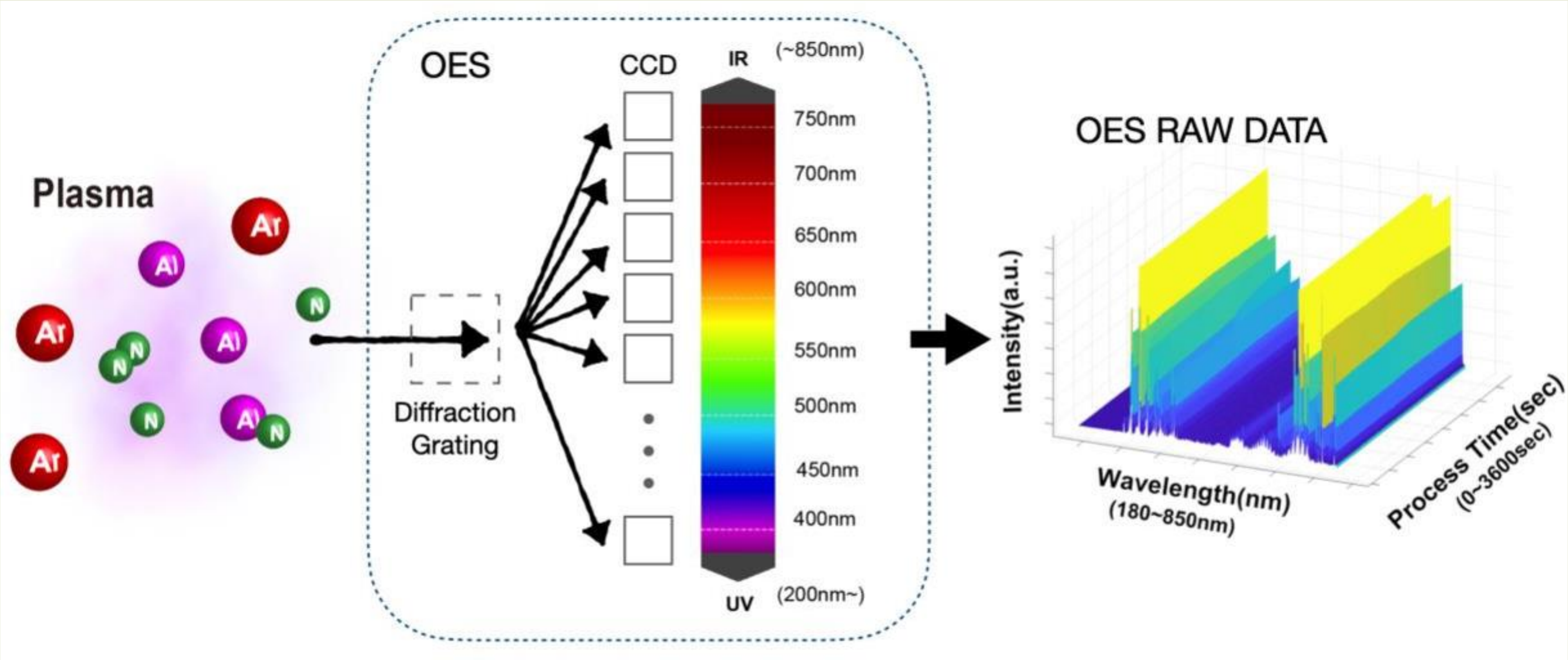
n_0 is total species population,

k_B is Boltzmann constant,

h is Planck constant and

c is speed of light.

Spectroscopy



https://www.semanticscholar.org/paper/Machine-Learning-Assisted-Classification-of-Nitride-Yang-Lu/02c3f186c326493f9480544824bdc282e9eb0999

OES spectra

OceanView 2.0.14 - Advance
File Window Help
Acquisition Group Window
OFX00893_1
Main Controls
Add/Remove Controls
Running
Data Update Rate 1 msec
Strobe/Lamp Enable:
Integration Time: Automatic
250 ms
Scans to Average: 30
Boxcar width: 2
No dark spectrum stored.
Store Now
Nonlinearity Correction:
Trigger Mode: On Demand
X-Axis: Wavelength (nm)
Throughput
Burst Mode
Spectrum back-to-back 1,000
Start
View Minus Bkgnd_5
Intensity (counts)
Wavelength (nm)
Subt_2:
Wavelengths (nm) 777,74
Subt_2: 21133,19
Schematic Window
View_2
OFX00893_1:
Wavelengths (nm) 656,422
OFX00893_1: 63052,65
OFX00893_1: 7500 msec
77%

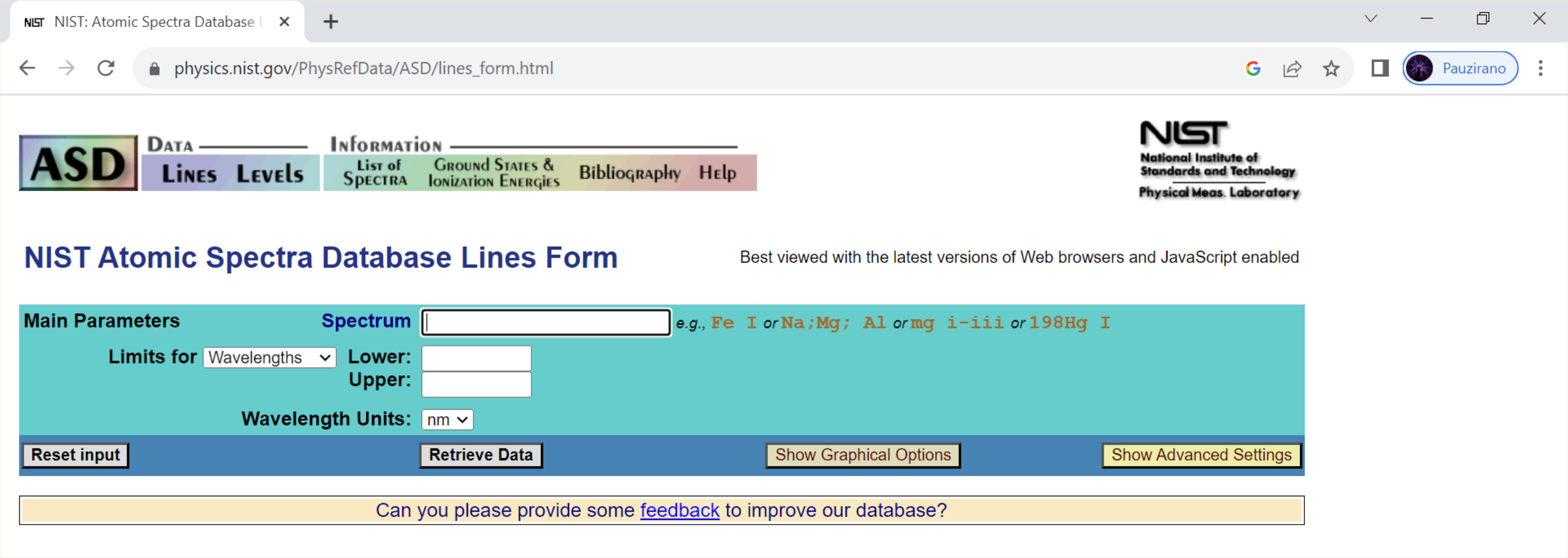
NIST

National Institute of Standards and Technology

Physical Meas. Laboratory

https://www.nist.gov/

is used for identification and confirmation of the spectral lines.



NIST ASD Output: Lines | /home/www/htdocs/PhysRefDat

physics.nist.gov/cgi-bin/ASD/lines1.pl?spectra=Ar&limits_type=0&low_w=350&upp_w=850&unit=1&submit=Retrieve+Data&de=0...

Pauzirano

ASD | Data: Lines | Levels | Information: List of Spectra | Ground States & Ionization Energies | Bibliography | Help

NIST National Institute of Standards and Technology Physical Meas. Laboratory

NIST Atomic Spectra Database Lines Data

Example of how to reference these results:
Kramida, A., Ralchenko, Yu., Reader, J., and NIST ASD Team (2022). *NIST Atomic Spectra Database* (ver. 5.10), [Online]. Available: https://physics.nist.gov/asd [2023, November 7]. National Institute of Standards and Technology, Gaithersburg, MD. DOI: https://doi.org/10.18434/T4W30F
BibTex Citation (new window)

Ar (all spectra): 1300 Lines of Data Found

Wavelength range: 350 - 850 nm
Wavelength in: vacuum below 200 nm, air between 200 and 2000 nm, vacuum above 2000 nm
Highest relative intensity: 35000

Query NIST Bibliographic Databases for **Ar** (new window)
Ar Energy Levels
Ar Line Wavelengths and Classification
Ar Transition Probabilities

Ion	Observed Wavelength Air (nm)	Unc. (nm)	Ritz Wavelength Air (nm)	Unc. (nm)	Rel. Int. (?)	A_{ki} (s^{-1})	Acc.	E_i (cm^{-1})		E_k (cm^{-1})	Lower Level Conf., Term, J			Upper Leve Conf., Term,	
Ar III	350.058	0.005	350.057415	0.000017	5	2.6e+07	D	196 590.6352	-	225 149.2072	$3s^2 3p^3 (^2D°) 4s$	$^3D°$	1	$3s^2 3p^3 (^2D°) 4p$	^3D
Ar III	350.26828	0.00001	350.268291	0.000016	93	4.3e+07	D	196 615.2125	-	225 156.5915	$3s^2 3p^3 (^2D°) 4s$	$^3D°$	2	$3s^2 3p^3 (^2D°) 4p$	^3D

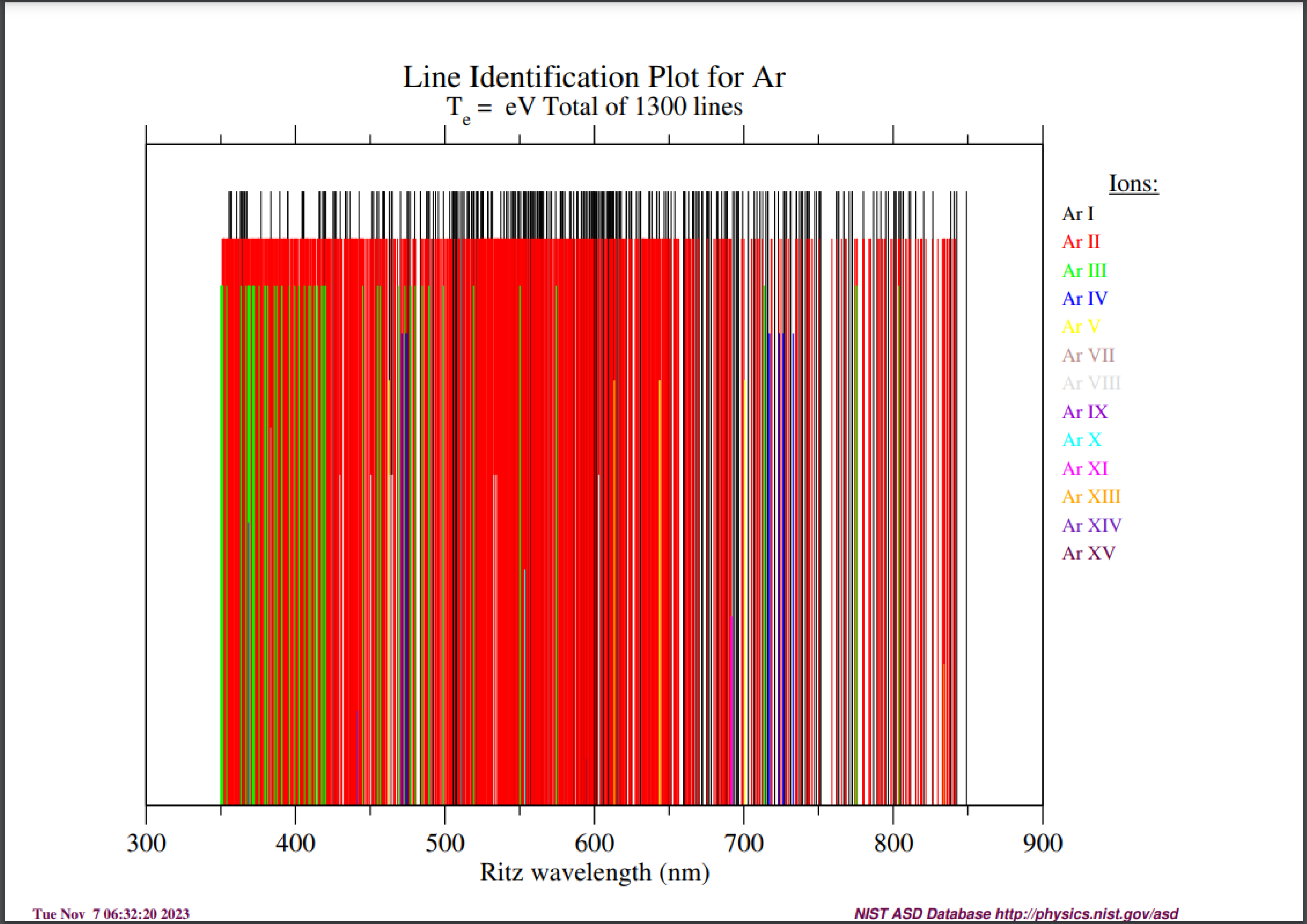
Range 350-850 nm

NIST ASD Output: Lines

physics.nist.gov/cgi-bin/ASD/lines1.pl?spectra=Ar&limits_type=0&low_w=350&upp_w=850&unit=1&submit=Retrieve+Data&de=0...

Ion	Observed Wavelength Air (nm)	Unc. (nm)	Ritz Wavelength Air (nm)	Unc. (nm)	Rel. Int. (?)	A_{ki} (s^{-1})	Acc.	E_i (cm^{-1})		E_k (cm^{-1})	Lower Level Conf., Term, J			Upper Level Conf., Term,
Ar III	350.058	0.005	350.057415	0.000017	5	2.6e+07	D	196 590.6352	-	225 149.2072	$3s^23p^3(^2D°)4s$	$^3D°$	1	$3s^23p^3(^2D°)4p$ ^3D
Ar III	350.26828	0.00001	350.268291	0.000016	93	4.3e+07	D	196 615.2125	-	225 156.5915	$3s^23p^3(^2D°)4s$	$^3D°$	2	$3s^23p^3(^2D°)4p$ ^3D
Ar III	350.35894	0.00001	350.358940	0.000014	468	1.2e+08	D	196 615.2125	-	225 149.2072	$3s^23p^3(^2D°)4s$	$^3D°$	2	$3s^23p^3(^2D°)4p$ ^3D
Ar III	350.93333	0.00001	350.933330	0.000017	245			180 678.3147	-	209 165.6077	$3s^23p^3(^4S°)4s$	$^3S°$	1	$3s^23p^3(^4S°)4p$ ^3P
Ar II	350.97779	0.00001	350.977794	0.000009	447	2.55e+08	B	155 708.1075	-	184 191.7917	$3s^23p^4(^3P)4p$	$^4P°$	$^1/_2$	$3s^23p^4(^3P)4d$ ^4D
Ar III	351.11485	0.00001	351.114850	0.000017	1175			180 678.3147	-	209 150.8807	$3s^23p^3(^4S°)4s$	$^3S°$	1	$3s^23p^3(^4S°)4p$ ^3P
Ar III	351.16671	0.00001	351.166713	0.000014	89	2.6e+07	D	196 680.8461	-	225 149.2072	$3s^23p^3(^2D°)4s$	$^3D°$	3	$3s^23p^3(^2D°)4p$ ^3D
Ar III	351.42004	0.00001	351.420041	0.000017	724			180 678.3147	-	209 126.1544	$3s^23p^3(^4S°)4s$	$^3S°$	1	$3s^23p^3(^4S°)4p$ ^3P
Ar II	351.43874	0.00001	351.438733	0.000005	490	1.36e+08	B	155 351.1206	-	183 797.4473	$3s^23p^4(^3P)4p$	$^4P°$	$^3/_2$	$3s^23p^4(^3P)4d$ ^4D
Ar II	351.78897	0.00010	351.788887	0.000007	4	7.e+04	E	132 630.7277	-	161 048.7411	$3s^23p^4(^3P)3d$	^4D	$^3/_2$	$3s^23p^4(^3P)4p$ ^4S
Ar II	351.893	0.004	351.8922	0.0014	1w,bl			190 592.2306	-	219 001.90	$3s^23p^4(^3P)4d$	^2P	$^3/_2$	$3s^23p^4(^1D_2)5f$ $^2[$
Ar II	351.99933	0.00001	351.999331	0.000004	191	5.2e+07	B	157 673.4134	-	186 074.4375	$3s^23p^4(^3P)4p$	$^4D°$	$^5/_2$	$3s^23p^4(^3P)4d$ ^4F
Ar II	352.12600	0.00001	352.125990	0.000005	100	2.27e+07	B	157 234.0196	-	185 624.8282	$3s^23p^4(^3P)4p$	$^4D°$	$^7/_2$	$3s^23p^4(^3P)4d$ ^4F

Range 350-850 nm



Range 600-700 nm

NIST ASD Output: Lines

physics.nist.gov/cgi-bin/ASD/lines1.pl?spectra=Ar&limits_type=0&low_w=600&upp_w=700&unit=1&submit=Retrieve+Data&de=0&lte_...

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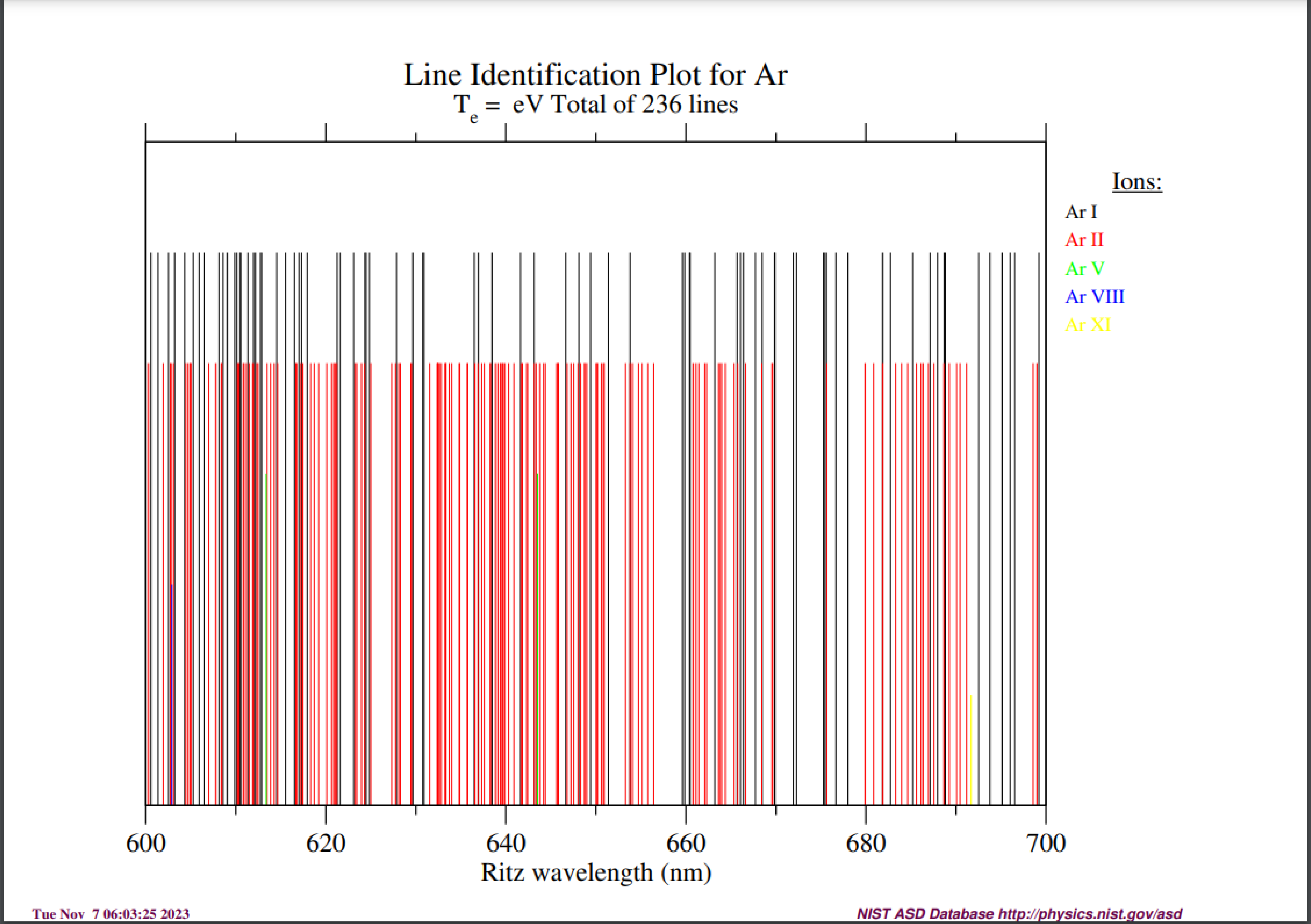
Ion	Observed Wavelength Air (nm)	Unc. (nm)	Ritz Wavelength Air (nm)	Unc. (nm)	Rel. Int. (?)	A_{ki} (s^{-1})	Acc.	E_i (cm^{-1})		E_k (cm^{-1})	Lower Level Conf., Term, J			Upper Level Conf., Term, J	
Ar II	600.3170	0.0008	600.31857	0.00006	1			158 167.7999	-	174 821.0098	$3s^23p^4(^3P)4p$	$^4D°$	$^3/_2$	$3s^23p^4(^1D)3d$	^2P
Ar I			600.5725	0.0010		1.4e+05	D+	107 289.7001	-	123 935.870	$3s^23p^5(^2P°_{1/2})4p$	$^2[^3/_2]$	2	$3s^23p^5(^2P°_{3/2})8s$	$^2[^3/_2]°$
Ar I			601.3677	0.0010		1.4e+05	D+	105 462.7596	-	122 086.9164	$3s^23p^5(^2P°_{3/2})4p$	$^2[^5/_2]$	3	$3s^23p^5(^2P°_{3/2})5d$	$^2[^3/_2]°$
Ar II	601.9493	0.0008	601.94965	0.00005	4			172 829.6539	-	189 437.7396	$3s^23p^4(^1D)3d$	^2D	$^3/_2$	$3s^23p^4(^3P)5p$	$^4P°$
Ar I	602.5150	0.0010	602.5150	0.0010	5	9.0e+05	D+	107 289.7001	-	123 882.203	$3s^23p^5(^2P°_{1/2})4p$	$^2[^3/_2]$	2	$3s^23p^5(^2P°_{1/2})7s$	$^2[^1/_2]°$
Ar II	602.72513	0.00007	602.72517	0.00003	7			173 347.9158	-	189 934.6322	$3s^23p^4(^1D)4p$	$^2D°$	$^3/_2$	$3s^23p^4(^3P)4d$	^2P
Ar II	602.8220	0.0008	602.823273	0.000015	1			190 511.2674	-	207 095.2846	$3s^23p^4(^3P)5p$	$^2D°$	$^5/_2$	$3s^23p^4(^3P)7s$	^4P
Ar VIII	602.98	0.08	602.9	0.4				1 070 277.	-	1 086 860.	$2p^69f$	$^2F°$	$^7/_2$	$2p^610g$	^2G
Ar II	603.0844	0.0008	603.08278	0.00004	1			191 169.5946	-	207 746.4757	$3s^23p^4(^3P)5p$	$^4S°$	$^3/_2$	$3s^23p^4(^3P)6d$	^4D
Ar I	603.2127	0.0010	603.2127	0.0010	70	2.46e+06	C	105 462.7596	-	122 036.0704	$3s^23p^5(^2P°_{3/2})4p$	$^2[^5/_2]$	3	$3s^23p^5(^2P°_{3/2})5d$	$^2[^7/_2]°$
Ar I	604.3223	0.0010	604.3223	0.0010	35	1.47e+06	C	105 617.2700	-	122 160.1502	$3s^23p^5(^2P°_{3/2})4p$	$^2[^5/_2]$	2	$3s^23p^5(^2P°_{3/2})5d$	$^2[^7/_2]°$
Ar II	604.4468	0.0008	604.44783	0.00009	7			192 712.058	-	209 251.5031	$3s^23p^4(^3P)4d$	^2D	$^3/_2$	$3s^23p^4(^1D_2)4f$	$^2[3]°$
Ar II	604.68977	0.00007	604.68967	0.00005	10			174 409.8916	-	190 942.7220	$3s^23p^4(^1D)3d$	^2P	$^3/_2$	$3s^23p^4(^3P)5p$	$^2S°$

Range 600-700 nm



Range 610-620 nm

NIST NIST ASD Output: Lines | /home/www/htdocs/PhysRefDat

physics.nist.gov/cgi-bin/ASD/lines1.pl?spectra=Ar&limits_type=0&low_w=610&upp_w=620&unit=1&submit=Retrieve+Data&de=0...

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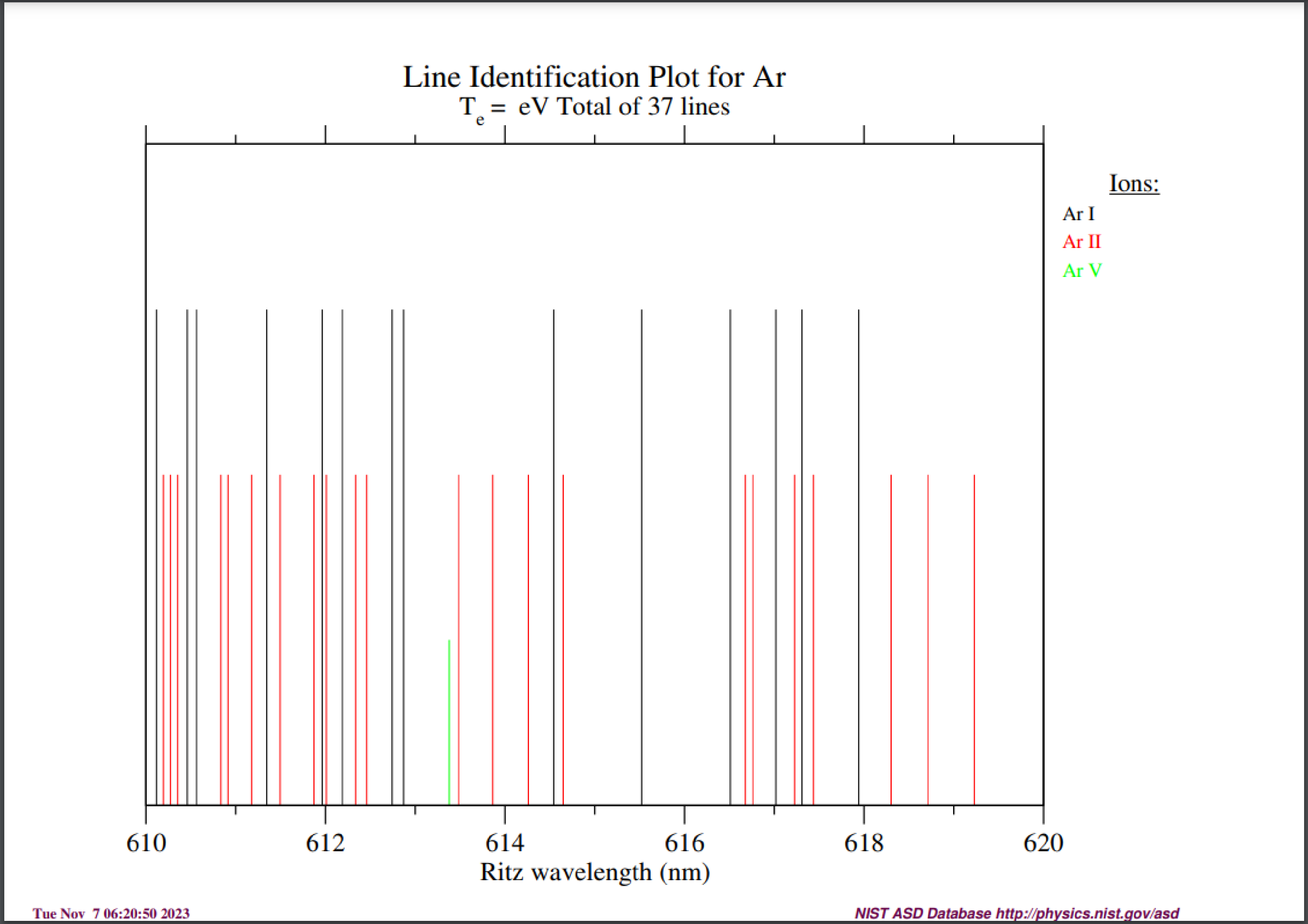
Ion	Observed Wavelength Air (nm)	Unc. (nm)	Ritz Wavelength Air (nm)	Unc. (nm)	Rel. Int. (?)	A_{ki} (s^{-1})	Acc.	E_i (cm^{-1})		E_k (cm^{-1})	Lower Level Conf., Term, J			Upper Level Conf., Term, J			Ty
Ar I			610.1161	0.0010		3.3e+05	D+	107 496.4166	-	123 882.203	$3s^23p^5(^2P^\circ_{1/2})4p$	$^2[^1/_2]$	1	$3s^23p^5(^2P^\circ_{1/2})7s$	$^2[^1/_2]^\circ$	1	
Ar II	610.19192	0.00007	610.19188	0.00005	4			179 931.8393	-	196 315.5916	$3s^23p^4(^1S)3d$	^2D	$^3/_2$	$3s^23p^4(^3P_1)4f$	$^2[3]^\circ$	$^5/_2$	
Ar II	610.2765	0.0008	610.274973	0.000012	1			186 816.0496	-	203 197.5711	$3s^23p^4(^3P)4d$	^2F	$^7/_2$	$3s^23p^4(^1D)5p$	$^2F^\circ$	$^7/_2$	
Ar II	610.35397	0.00005	610.353914	0.000015	26	1.7e+06	C	144 709.9818	-	161 089.3846	$3s^23p^4(^3P)3d$	^2P	$^1/_2$	$3s^23p^4(^3P)4p$	$^2S^\circ$	$^1/_2$	
Ar I			610.4590	0.0010		3.4e+05	D	107 496.4166	-	123 873.000	$3s^23p^5(^2P^\circ_{1/2})4p$	$^2[^1/_2]$	1	$3s^23p^5(^2P^\circ_{1/2})7s$	$^2[^1/_2]^\circ$	0	
Ar I	610.5635	0.0010	610.5635	0.0010	10	1.21e+06	C	107 131.7086	-	123 505.4896	$3s^23p^5(^2P^\circ_{1/2})4p$	$^2[^3/_2]$	1	$3s^23p^5(^2P^\circ_{1/2})5d$	$^2[^5/_2]^\circ$	2	
Ar II	610.832	0.002	610.83261	0.00006	0?			192 556.9179	-	208 923.4846	$3s^23p^4(^3P)4d$	^2D	$^5/_2$	$3s^23p^4(^1D_2)4f$	$^2[2]^\circ$	$^3/_2$	
Ar II	610.915	0.002	610.91548	0.00006	2p			192 556.9179	-	208 921.2645	$3s^23p^4(^3P)4d$	^2D	$^5/_2$	$3s^23p^4(^1D_2)4f$	$^2[2]^\circ$	$^5/_2$	
Ar II	611.1742	0.0008	611.1744	0.0003	2			192 556.9179	-	208 914.333	$3s^23p^4(^3P)4d$	^2D	$^5/_2$	$3s^23p^4(^3P_2)7p$	$^2[2]^\circ$	$^5/_2$	
Ar I			611.3466	0.0010		4.7e+04	D+	106 087.2598	-	122 440.0672	$3s^23p^5(^2P^\circ_{3/2})4p$	$^2[^3/_2]$	1	$3s^23p^5(^2P^\circ_{3/2})7s$	$^2[^3/_2]^\circ$	2	
Ar II	611.49232	0.00001	611.492319	0.000015	537	2.00e+07	B+	154 181.4942	-	170 530.4040	$3s^23p^4(^1D)3d$	^2G	$^9/_2$	$3s^23p^4(^1D)4p$	$^2F^\circ$	$^7/_2$	
Ar II	611.8724	0.0008	611.872214	0.000015	4	1.e+05	E	144 709.9818	-	161 048.7411	$3s^23p^4(^3P)3d$	^2P	$^1/_2$	$3s^23p^4(^3P)4p$	$^4S^\circ$	$^3/_2$	
Ar I			611.9656	0.0010		5.1e+04	D+	107 131.7086	-	123 467.9733	$3s^23p^5(^2P^\circ_{1/2})4p$	$^2[^3/_2]$	1	$3s^23p^5(^2P^\circ_{3/2})6d$	$^2[^1/_2]^\circ$	1	

Range 610-620 nm



Role of machine learning for optical emission spectroscopy

The emphasis of mentioned models is the **identification of major production and depopulation processes under different plasma discharge conditions and for different kinds of excited species**.

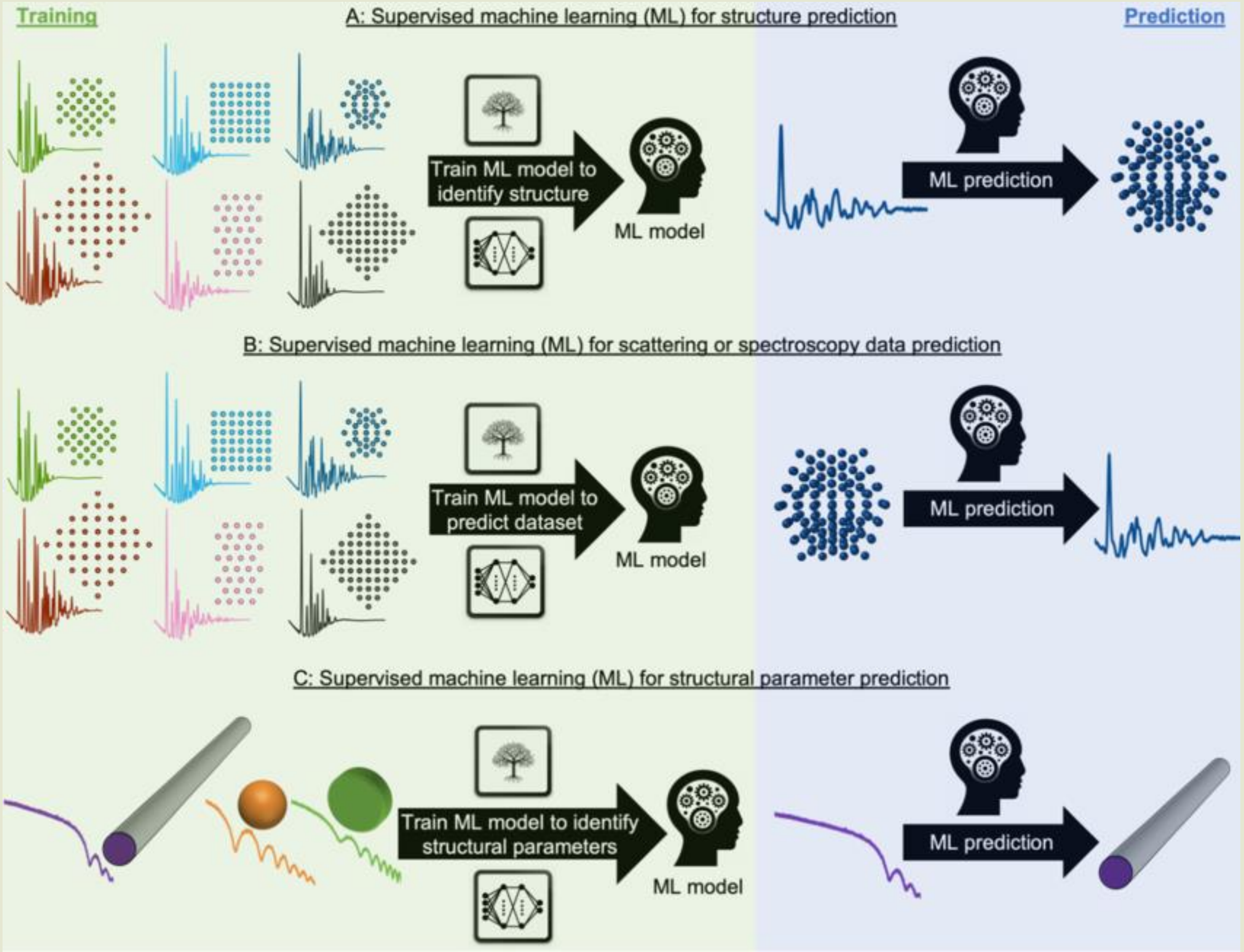
The quality of the modelling results, which determines the accuracy of diagnostic results by the line intensity ratio method, depends on the existence and quality of the data used.

The line intensity ratio method is expected to be further developed in the future.

Many studies have demonstrated the **effectiveness of ML for OES**.

ML for OES

The fundamental idea in ML is that, for many applications, **training a computer algorithm for predicting or finding patterns in the behavior of a complex system by observing many input–output samples** of its behavior can be significantly simpler than developing physics-based models.



https://www.researchgate.net/figure/A-Use-of-ML-for-identifying-a-structural-model-During-training-a-supervised-ML-model_fig1_373530521

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Thank you for your attention!

UNIVERSITY OF ZAGREB

Faculty of Electrical Engineering and Computing

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