Consiglio Nazionale delle Ricerche
istec Istituto di Scienza e Tecnologia dei Materiali Ceramici

Assessment of Cytotoxicity of Metal Oxide Nanoparticles on the Basis of Immediately Available Physical-Chemical Parameters

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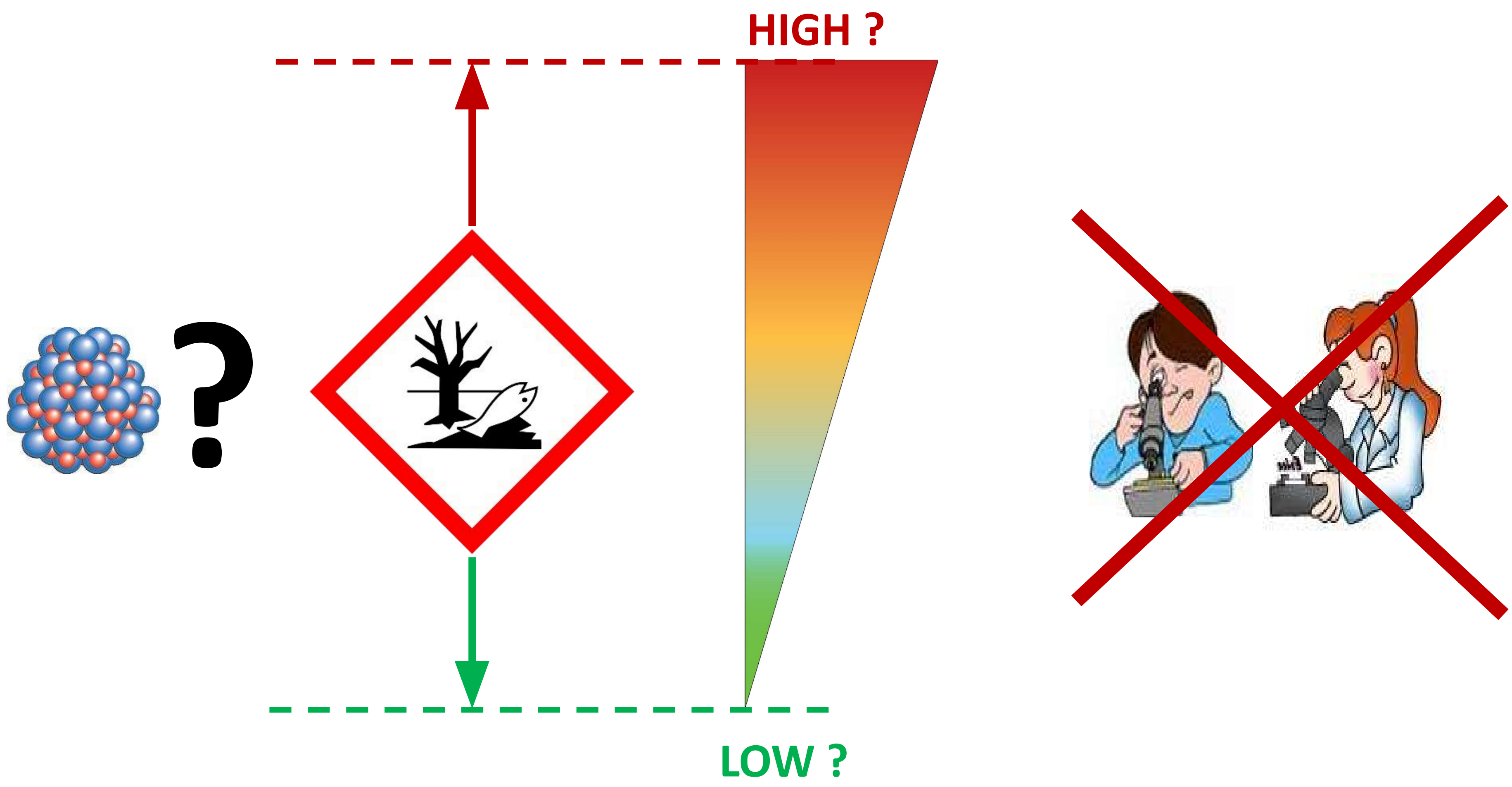
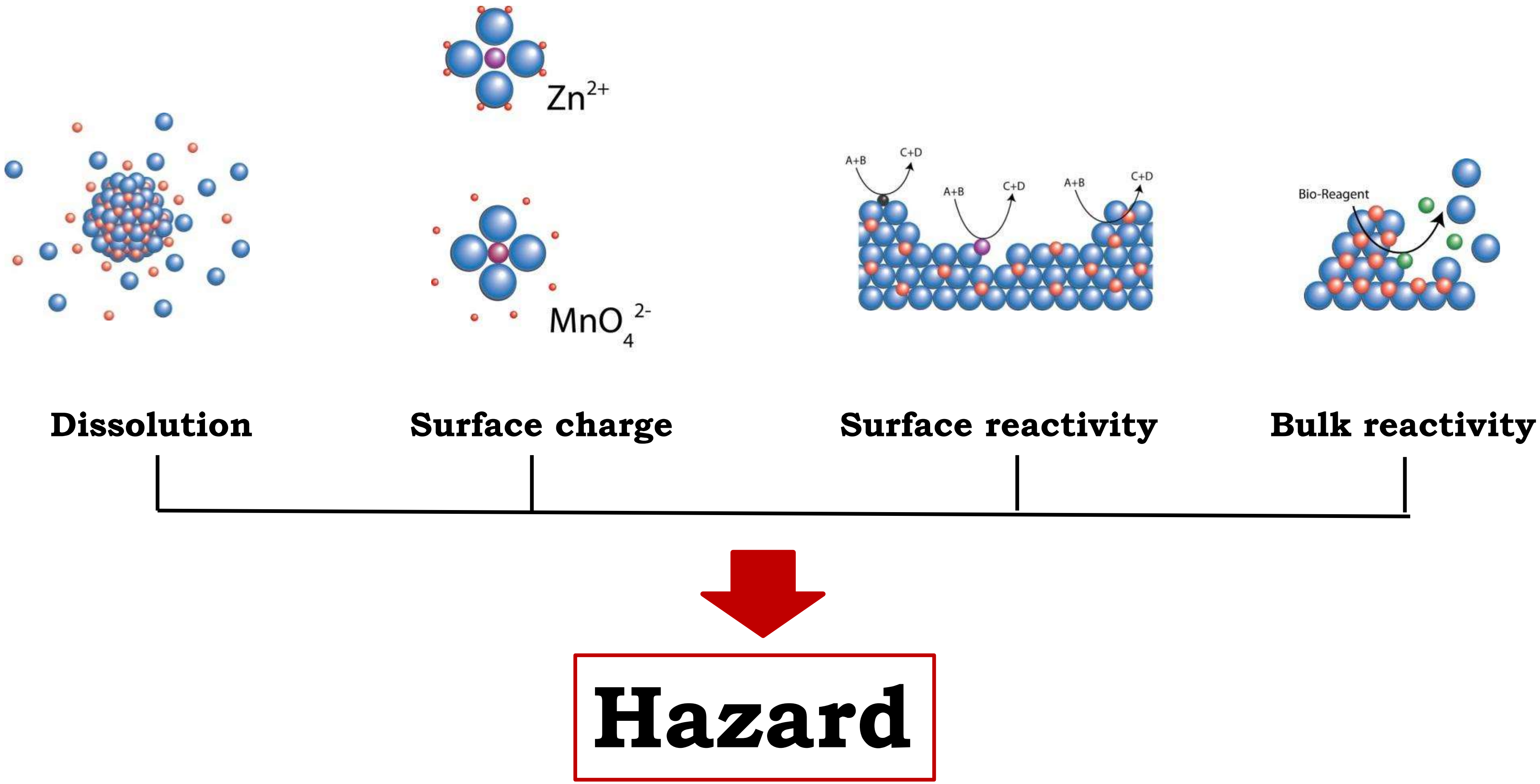
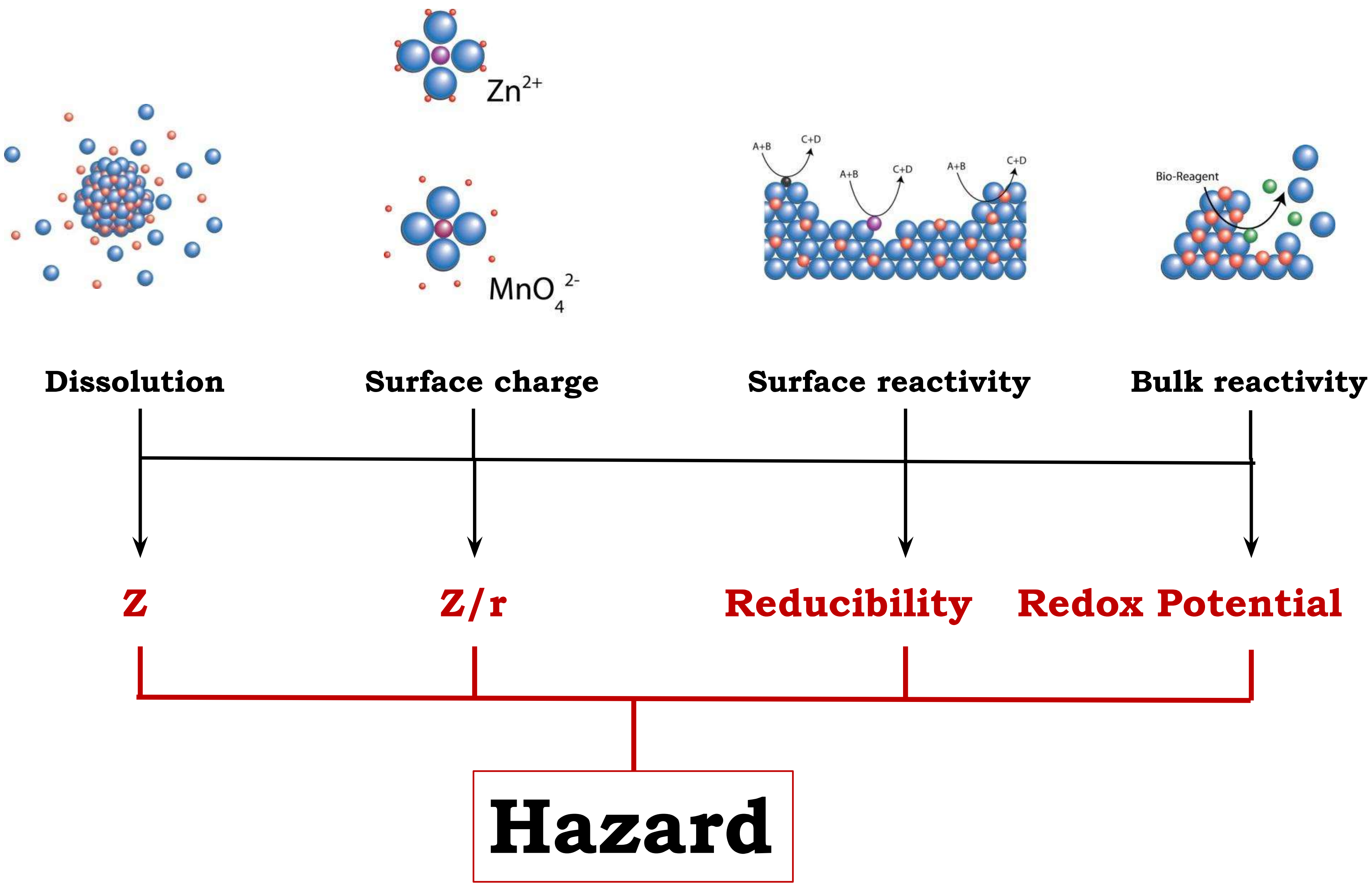
Hazard of a Nanoparticle Before Running any Experiment

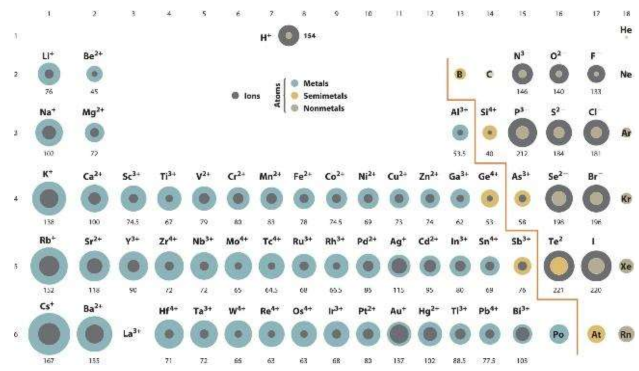




Zn2+
MnO4 2-
A+B
C+D
Bio-Reagent
Dissolution
Surface charge
Surface reactivity
Bulk reactivity
Hazard



Zn^{2+}
MnO_4^{2-}
A+B
C+D
Bio-Reagent
Dissolution
Surface charge
Surface reactivity
Bulk reactivity
Z
Z/r
Reducibility
Redox Potential
Hazard



Z

Oxidation number
given by the Chemical Formula

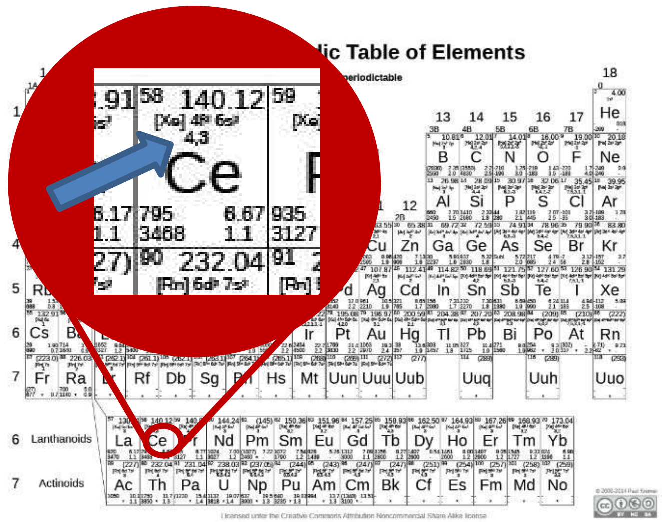
Ionic Potential = Z/r

Ionic Radii Measured in the '30
(Available on the Internet)

Hazard

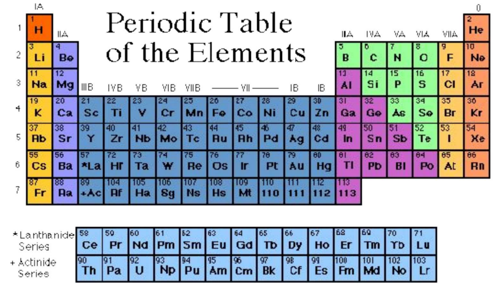
Reducibility deduced
from a Periodic Table

Redox Potential
available everywhere

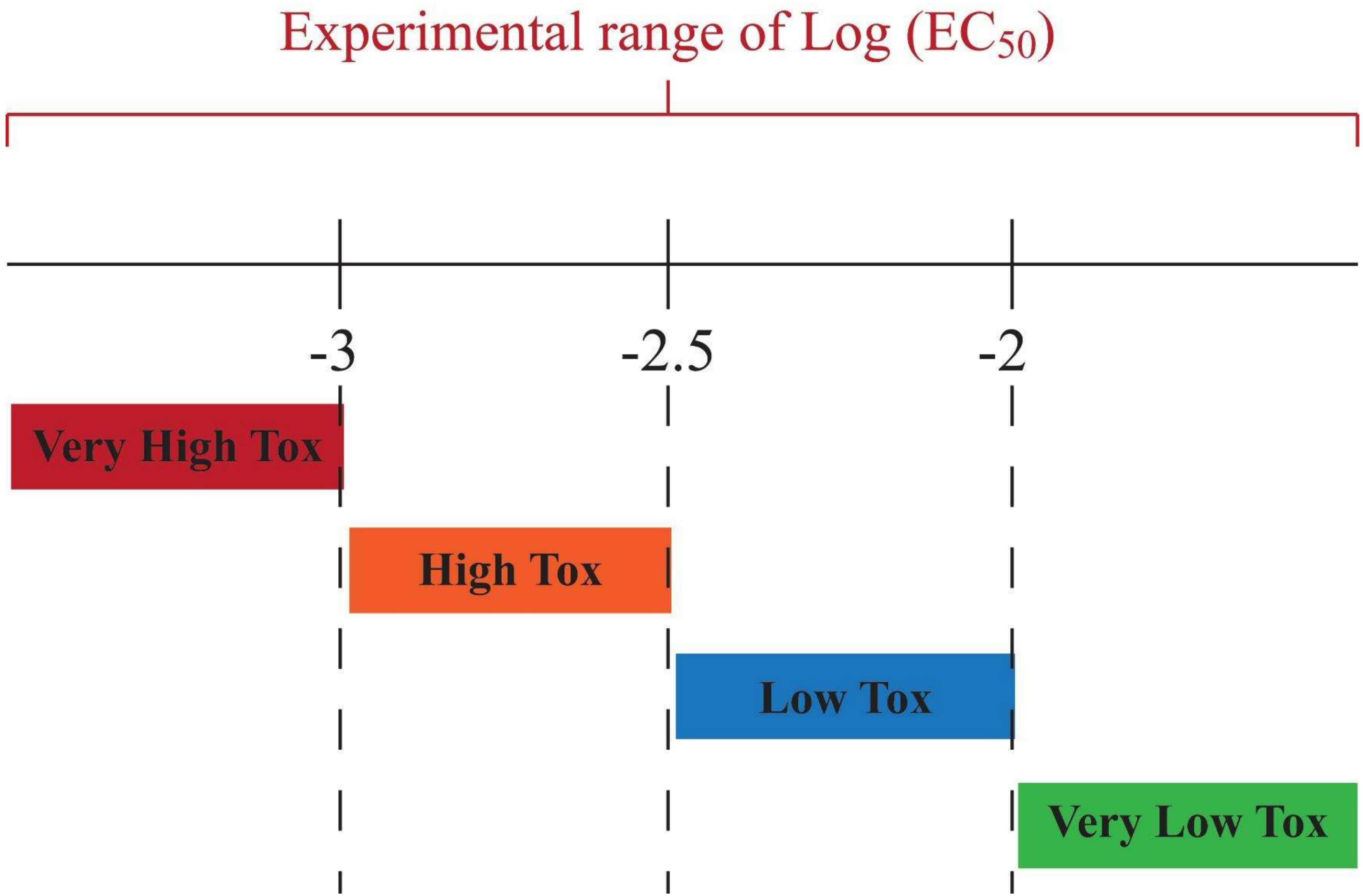


Reaction	Log K at 25°C	Standard Electrode Potential (V) at 25°C
$Na^+ + e^- = Na(s)$	−46	−2.71
$Mg^{2+} + 2e^- = Mg(s)$	−79.7	−2.35
$Zn^{2+} + 2e^- = Zn(s)$	−26	−0.76
$Fe^{2+} + 2e^- = Fe(s)$	−14.9	−0.44
$Co^{2+} + 2e^- = Co(s)$	−9.5	−0.28
$V^{3+} + e^- = V^{2+}$	−4.3	−0.26
$2H^+ + 2e^- = H_2(g)$	0.0	0.00
$S(s) + 2H^+ + 2e^- = H_2S$	+4.8	+0.14
$Cu^{2+} + e^- = Cu^+$	+2.7	+0.16
$AgCl(s) + e^- = Ag(s) + Cl^-$	+3.7	+0.22
$Cu^{2+} + 2e^- = Cu(s)$	+11.4	+0.34
$Cu^+ + e^- = Cu(s)$	+8.8	+0.52
$Fe^{3+} + e^- = Fe^{2+}$	+13.0	+0.77
$Ag^+ + e^- = Ag(s)$	+13.5	+0.80
$Fe(OH)_3(s) + 3H^+ + e^- = Fe^{2+} + 3H_2O$	+17.1	+1.01
$IO_3^- + 6H^+ + 5e^- = \frac{1}{2}I_2(s) + 3H_2O$	+104	+1.23
$MnO_2(s) + 4H^+ + 2e^- = Mn^{2+} + 2H_2O$	+43.6	+1.29
$Cl_2(g) + 2e^- = 2Cl^-$	+46	+1.36
$Co^{3+} + e^- = Co^{2+}$	+31	+1.82

Risk
Assessment



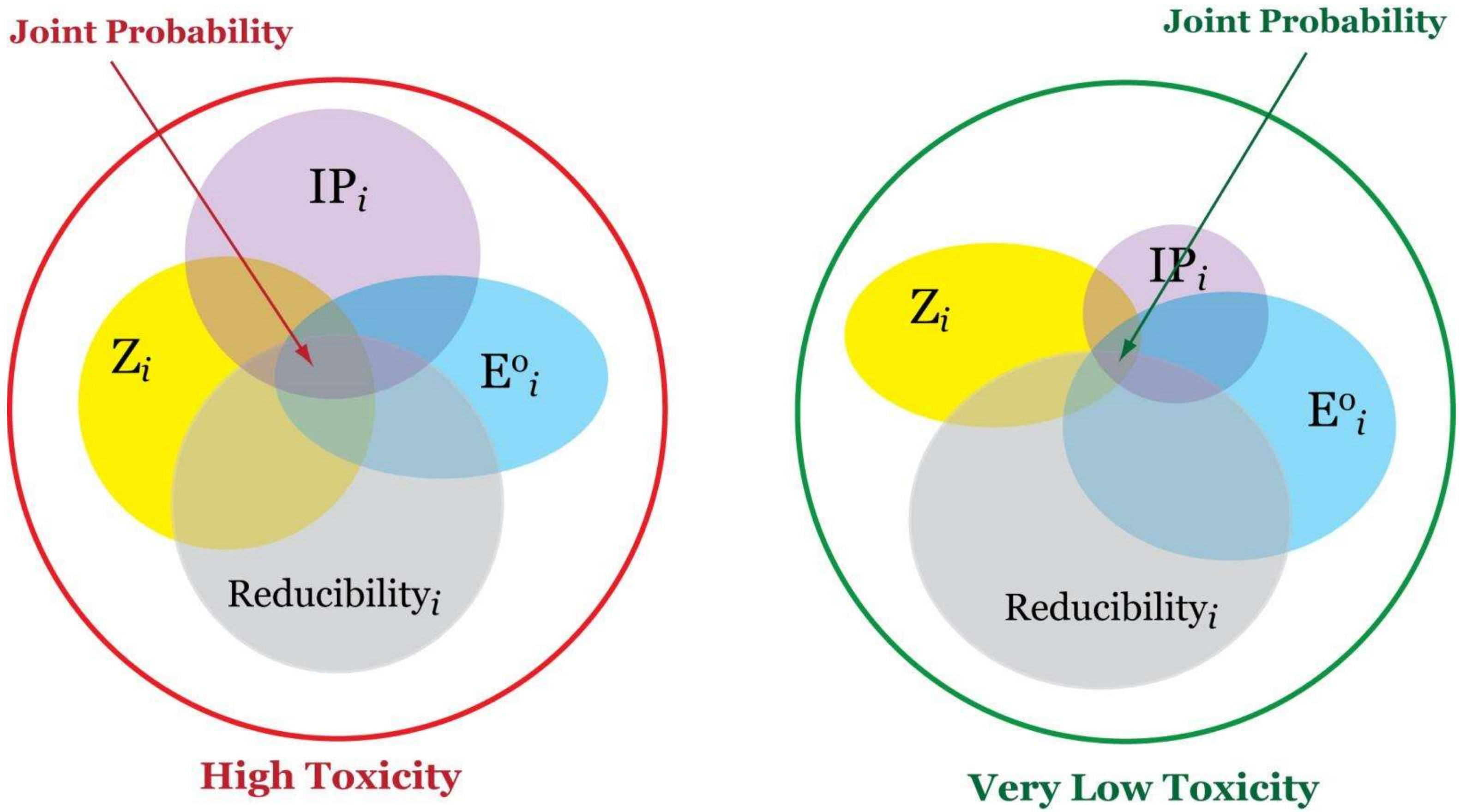
Definition of classes of toxicity



Oxide	Oxidation Number Z	Ionic Potential IP	Surface Reducibility SR	Redox Reactivity RR	Class of Toxicity (Experimental)
ZnO	≤ 2	≤ 3	Non Reducible	Non Active	Very high toxicity
NiO	≤ 2	≤ 3	Oxidizable	Active	Very high toxicity
Mn_2O_3	3	> 5	Oxidizable	Active	Very high toxicity
Cr_2O_3	3	3-5	Oxidizable	Active	High toxicity
Y_2O_3	3	3-5	Reducible	Non Active	High toxicity
Bi_2O_3	3	≤ 3	Oxidizable	Active	High toxicity
MoO_3	> 4	> 5	Reducible	Active	High toxicity
Gd_2O_3	3	≤ 3	Reducible	Non Active	High toxicity
V_2O_3	3	3-5	Oxidizable	Active	High toxicity
ZrO_2	≥ 4	> 5	Reducible	Non Active	Low toxicity
Al_2O_3	3	> 5	Reducible	Non Active	Low toxicity
TiO_2	≥ 4	> 5	Reducible	Non Active	Very low toxicity
SiO_2	≥ 4	> 5	Non reducible	Non Active	Very low toxicity
HfO_2	≥ 4	> 5	Reducible	Non Active	Very low toxicity
WO_3	≥ 4	> 5	reducible	Non Active	Very low toxicity

Naive Bayes Classifier

Most probable level of toxicity of $NP_i = [Z_i, IP_i, SR_i, RR_i]$?



$$P(Tox|NP_i) \propto P(Z_i|Tox) \times P(IP_i|Tox) \times P(SR_i|Tox) \times P(RR_i|Tox)$$

ZnO $Z \leq 2$ $IP \leq 3$ Non Reducible Non Active

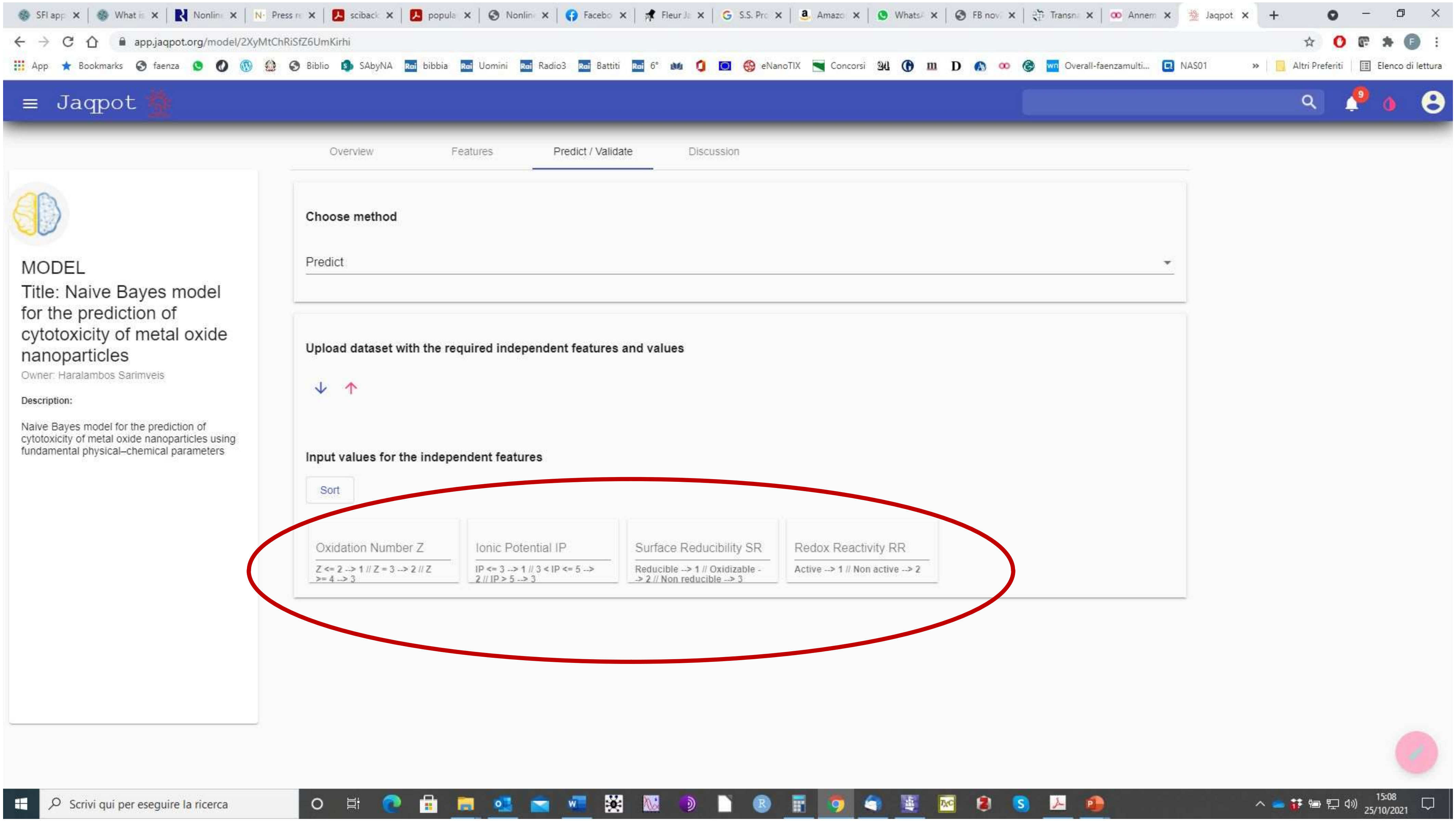
Z **Oxidation Number**	**IP** **Ionic Potential**	**SR** **Surface Reducibility**	**RR** **Redox Reactivity**
$P(Z \leq 2 \mid VT) = 0.666$	$P(IP \leq 3 \mid VT) = 0.666$	$P(SR=NR \mid VT) = 0.333$	$P(RR=A^{d} \mid VT) = 0.665$
$P(Z \leq 2 \mid HT) = 0.001$*	$P(IP \leq 3 \mid HT) = 0.333$	$P(SR=NR \mid HT) = 0.001$*	$P(RR=A \mid HT) = 0.665$
$P(Z \leq 2 \mid LT) = 0.001$*	$P(IP \leq 3 \mid LT) = 0.001$*	$P(SR=NR \mid LT) = 0.001$*	$P(RR=A \mid LT) = 0.001$*
$P(Z \leq 2 \mid VL) = 0.001$*	$P(IP \leq 3 \mid VL) = 0.001$*	$P(SR=NR \mid VL) = 0.249$	$P(RR=A \mid VL) = 0.001$*
$P(Z=3 \mid VT) = 0.333$	$P(IP=3\text{-}5 \mid VT) = 0.001$*	$P(SR=R^{b} \mid VT) = 0.001$*	$P(RR=NA \mid VT)=0.335$
$P(Z=3 \mid HT) = 0.833$	$P(IP=3\text{-}5 \mid HT) = 0.501$	$P(SR=R \mid HT) = 0.500$	$P(RR=NA \mid HT)=0.335$
$P(Z=3 \mid LT) = 0.500$	$P(IP=3\text{-}5 \mid LT) = 0.001$*	$P(SR=R \mid LT) = 0.998$	$P(RR=NA \mid LT)=0.999$
$P(Z=3 \mid VL) = 0.001$*	$P(IP=3\text{-}5 \mid VL) = 0.001$*	$P(SR=R \mid VL) = 0.750$	$P(RR=NA \mid VL)=0.999$
$P(Z \geq 4 \mid VT) = 0.001$*	$P(IP>5 \mid VT) = 0.333$	$P(SR=O^{c} \mid VT) = 0.666$	
$P(Z \geq 4 \mid HT) = 0.166$	$P(IP>5 \mid HT) = 0.166$	$P(SR=O \mid HT) = 0.499$	
$P(Z \geq 4 \mid LT) = 0.499$	$P(IP>5 \mid LT) = 0.998$	$P(SR=O \mid LT) = 0.001$*	
$P(Z \geq 4 \mid VL) = 0.998$	$P(IP>5 \mid VL) = 0.998$	$P(SR=O \mid VL) = 0.001$*	

P(ZnO|VT) = 0.666 x 0.666 x 0.333 x 0.335 = **0.05**

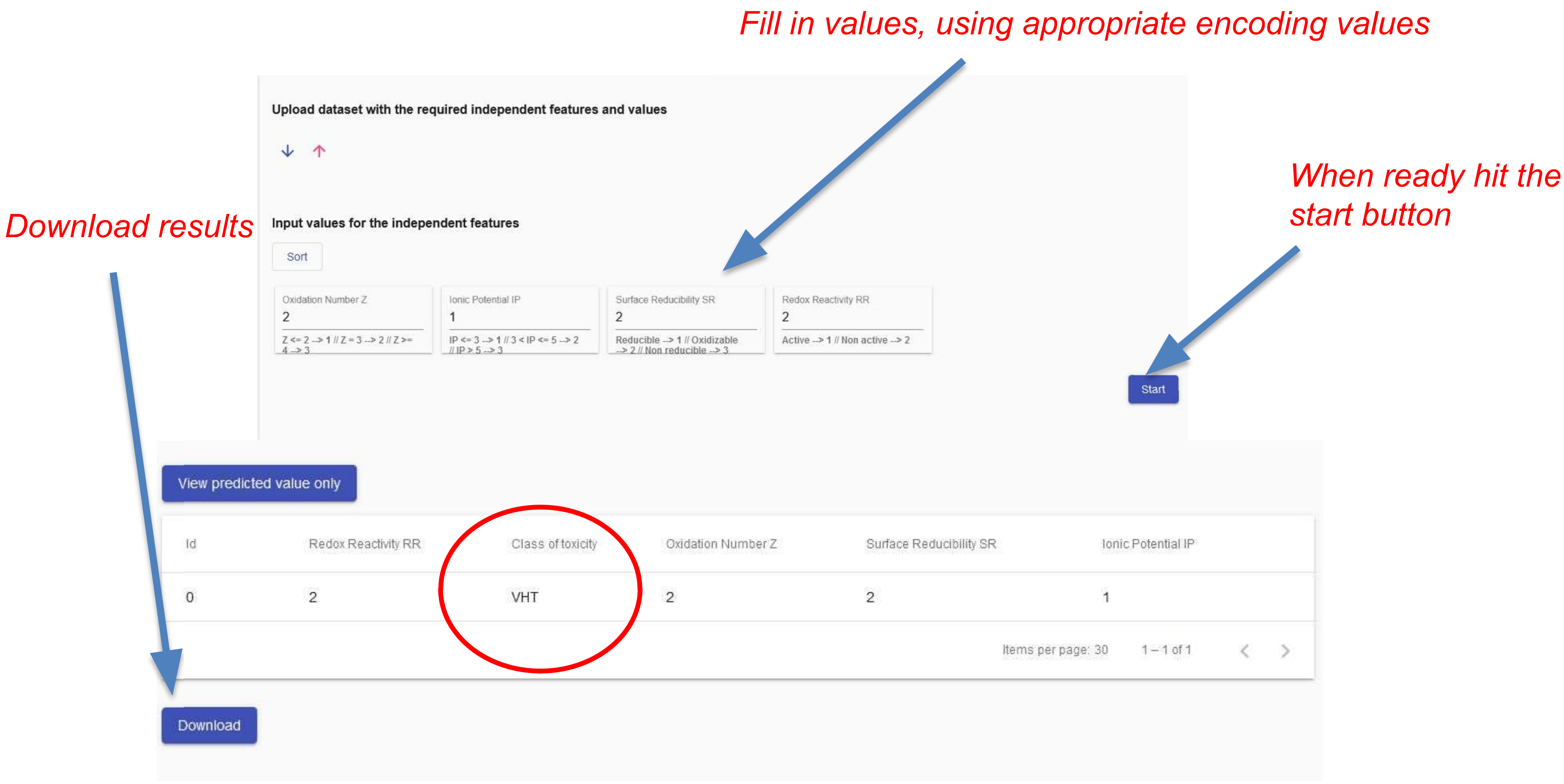
P(ZnO|HT) = 0.001 x 0.333 x 0.001 x 0.335 = **0.0000005**

P(ZnO|LT) = 0.001 x 0.001 x 0.001 x 0.999 = **0.000000001**

P(ZnO|VT) = 0.001 x 0.001 x 0.249 x 0.299 =**0.00000007**

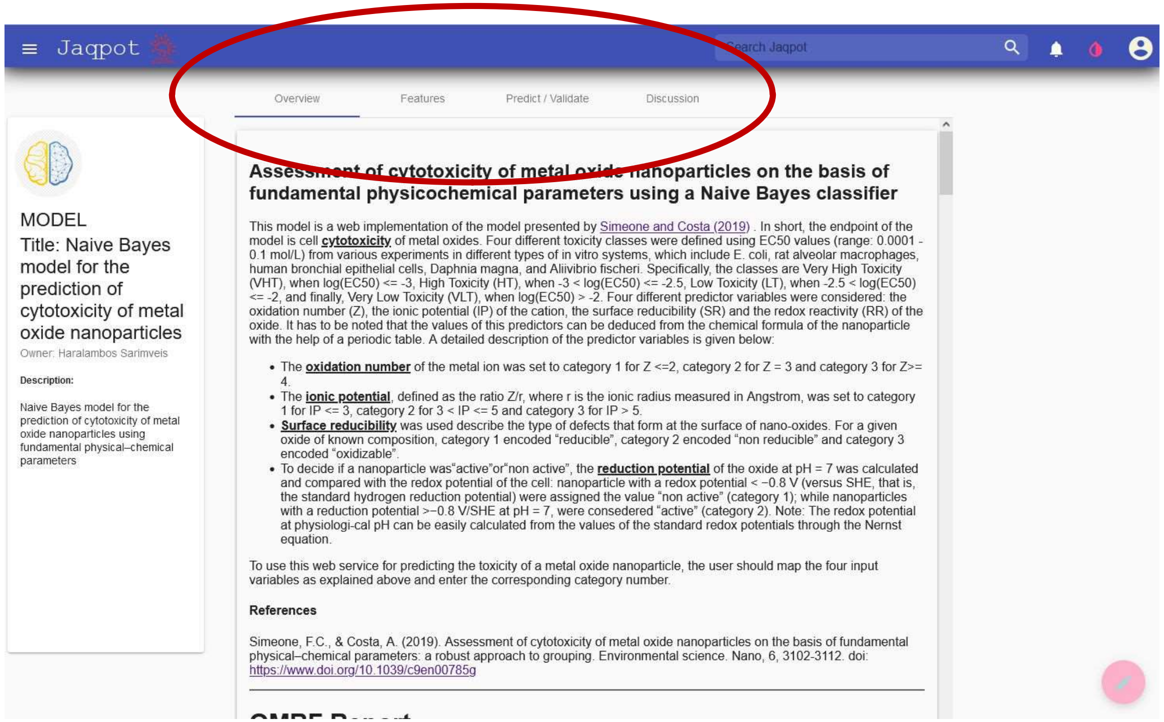


app.jaqpot.org/model/2XyMtChRiSfZ6UmKirhi
Jaqpot
Overview
Features
Predict / Validate
Discussion
MODEL
Title: Naive Bayes model for the prediction of cytotoxicity of metal oxide nanoparticles
Owner: Haralambos Sarimveis
Description:
Naive Bayes model for the prediction of cytotoxicity of metal oxide nanoparticles using fundamental physical–chemical parameters
Choose method
Predict
Upload dataset with the required independent features and values
Input values for the independent features
Sort
Oxidation Number Z
Z <= 2 --> 1 // Z = 3 --> 2 // Z >= 4 --> 3
Ionic Potential IP
IP <= 3 --> 1 // 3 < IP <= 5 --> 2 // IP > 5 --> 3
Surface Reducibility SR
Reducible --> 1 // Oxidizable --> 2 // Non reducible --> 3
Redox Reactivity RR
Active --> 1 // Non active --> 2
Scrivi qui per eseguire la ricerca
15:08
25/10/2021

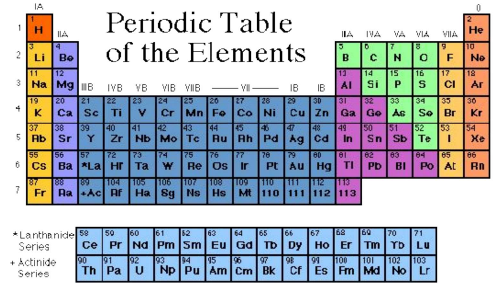

Fill in values, using appropriate encoding values
When ready hit the start button
Download results
Upload dataset with the required independent features and values
Input values for the independent features
Sort
Oxidation Number Z
2
Z <= 2 --> 1 // Z = 3 --> 2 // Z >= 4 --> 3
Ionic Potential IP
1
IP <= 3 --> 1 // 3 < IP <= 5 --> 2 // IP > 5 --> 3
Surface Reducibility SR
2
Reducible --> 1 // Oxidizable --> 2 // Non reducible --> 3
Redox Reactivity RR
2
Active --> 1 // Non active --> 2
Start
View predicted value only
Id
Redox Reactivity RR
Class of toxicity
Oxidation Number Z
Surface Reducibility SR
Ionic Potential IP
0
2
VHT
2
2
1
Items per page: 30
1 – 1 of 1
Download

Model Page Tabs

- ‘***Overview***’ contains information on the model;
- ‘***Features***’ documents the encoding and units of the features;
- ‘***Predict/Validate*** ’ allows prediction and validation of the model;
- ‘***Discussion***’ allows end-users to leave comments, thoughts and ideas on the model;



Risk Assessment



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