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Please pay attention to your time limit!

Every speaker must introduce the next speaker (name, surname and title)

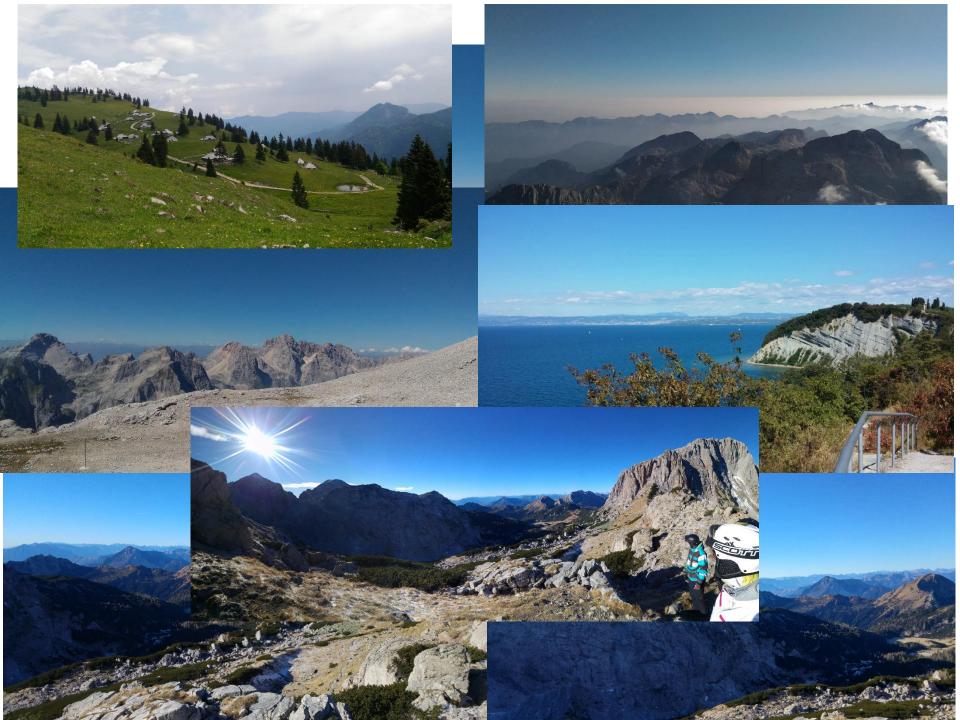
Pitches will be graded by a jury composed of professors and public

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Earth, how old are you?

Leja Rovan Department of Environmental Sciences, Jožef Stefan Institute Poster number: 39



Radiometric dating

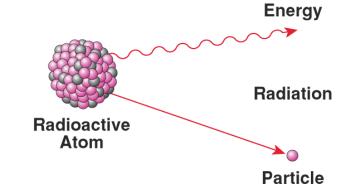
Radiometric dating

Radioactive process

238

Unstable isotope

Uranium – lead dating:



²⁰⁶Pb

Stable isotope

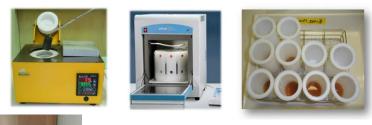
 $t_{1/2} = 4.47 \times 10^9$ years

Mineral zircon:



Analytical procedure

- Sample preparation
 - Pre-concentration or digestion
 - Chemical separation



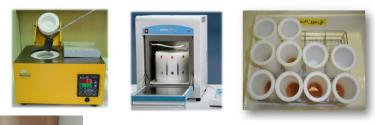


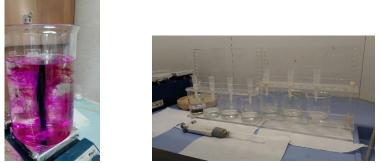
- Measurement
 - ✤ Multi-collector inductively coupled plasma mass spectrometry → MC-ICP-MS



Analytical procedure

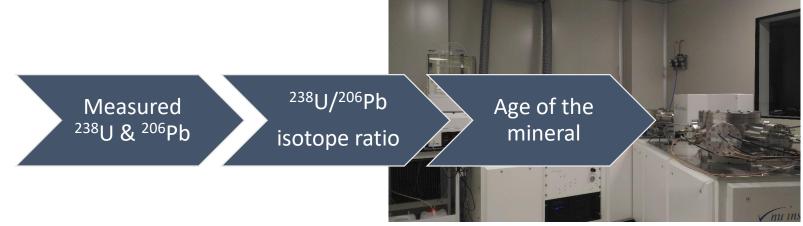
- Sample preparation
 - Pre-concentration or digestion
 - Chemical separation



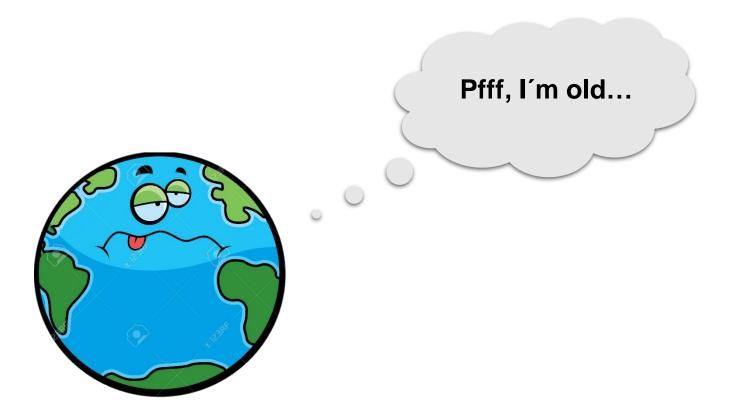


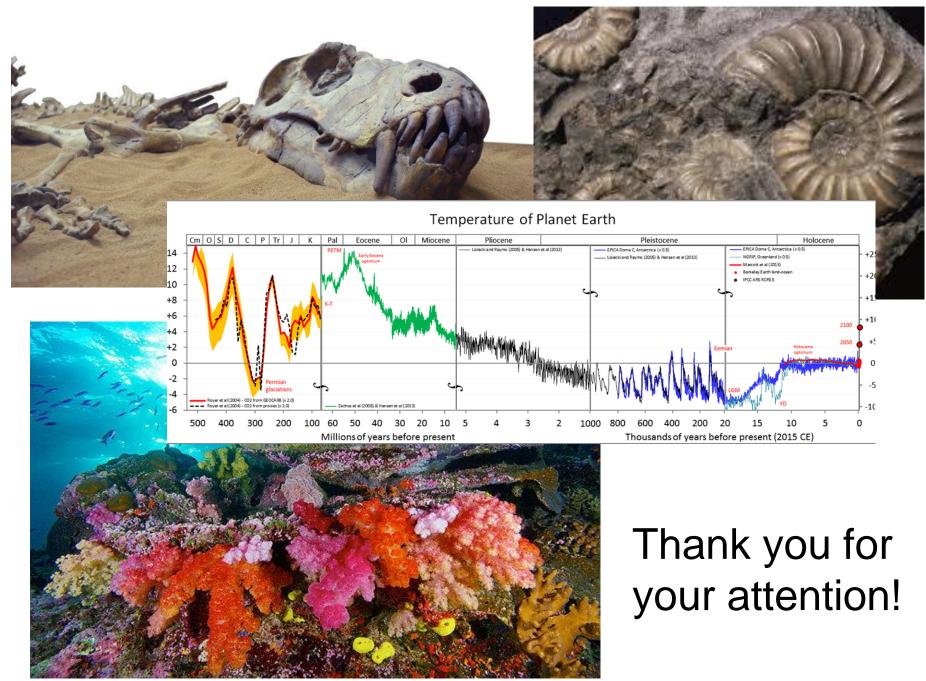
Measurement

✤ Multi-collector inductively coupled plasma mass spectrometry → MC-ICP-MS



Age of the earth: 4.54 billion years!





Picture reference: Internet

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Neurodegenerative Diseases Data Ontology

Ana Kostovska, Ilin Tolovski

Department of Knowledge Technologies, Jožef Stefan Institute, Ljubljana, Slovenia

Jožef Stefan International Postgraduate School, Ljubljana, Slovenia

Poster number: 7

Introduction

- Heterogeneous group of disorders that are characterized by the progressive degeneration of the structure and function of the central nervous system or peripheral nervous system
 - Alzheimer's disease Irreversible neurodegenerative disease that results in a loss of mental function due to the deterioration of brain tissue
 - Parkinson's disease Disorder of the central nervous system that results from the loss of cells in various parts of the brain, categorized as a movement disorder
- Ontology
 - A set of concepts and categories in a subject area or domain that shows their properties and the relations between them





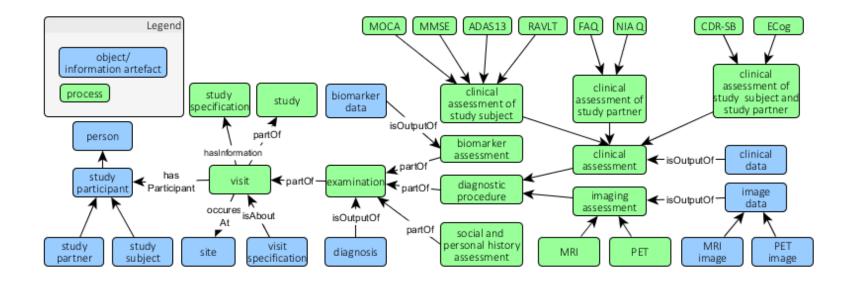
Motivation

- Large number of clinical studies of neurodegenerative diseases
- Need for a unified representation of the neurodegenerative diseases data originating from different studies (or hospitals)
- We adressed the task of designing and implementing an ontology for describing data on patients with neurodegenerative diseases
- Having an ontology for describing data on patients is important from two different perspectives:
 - from a viewpoint of ontology-based data access (ODBA) it would allow federation queries on data produced and stored at different hospitals;
 - from viewpoint of data analytics it would allow (semi) automatic creation of data analysis workflows based on the datatypes that occur in the datasets, annotated with ontology terms.





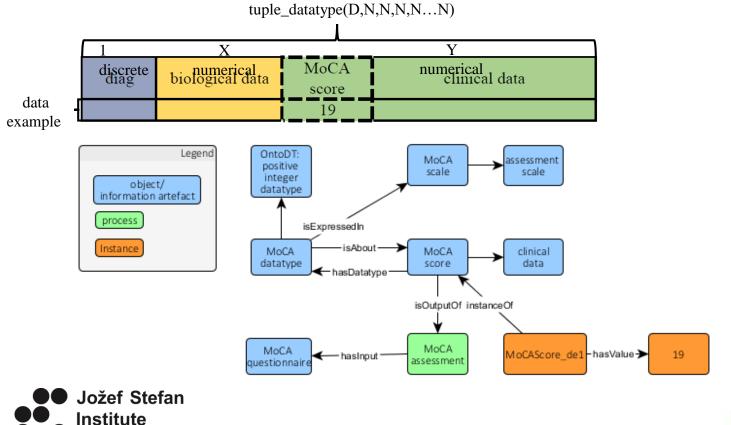
NDDO basic scheme







Example of semantic annotation



Ljubljana, Slovenija



Thank you for your attention!

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Can magnets be a cure for cancer?

Effect of barium-hexaferrite nanoplatelets in low-frequency magnetic field on cancer cells

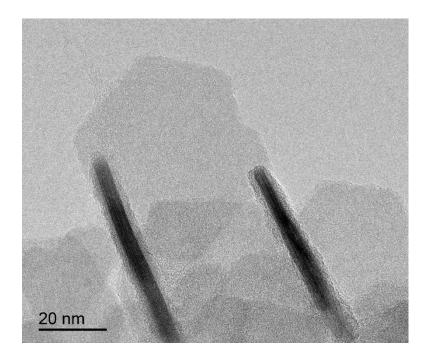
Tanja Goršak,

Department for Materials Synthesis, Jožef Stefan Institute

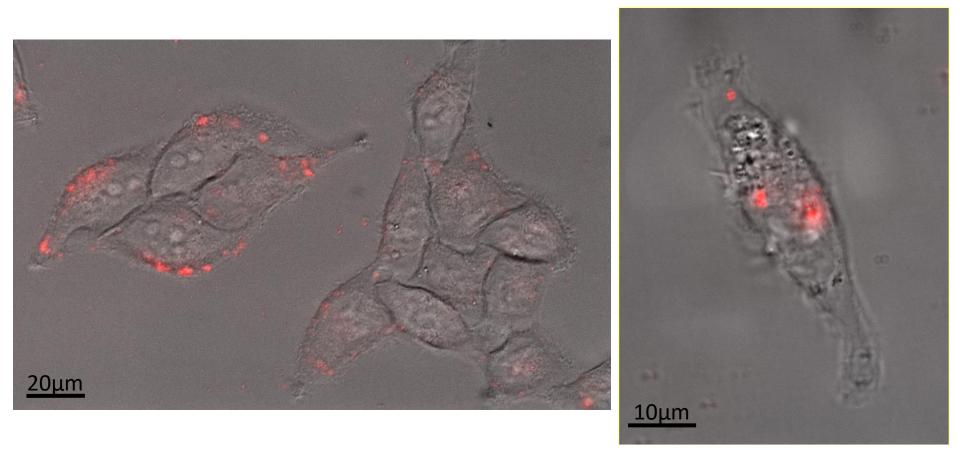
Poster number: 29

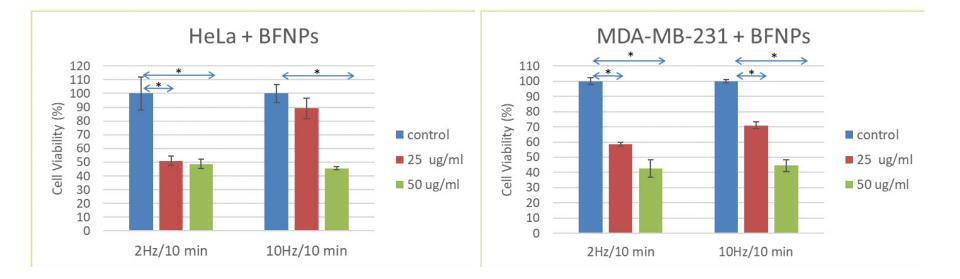












Thank you for your attention

Questions: Poster 29

Email: tanja.gorsak@ijs.si



Now Bring Me That Horizon

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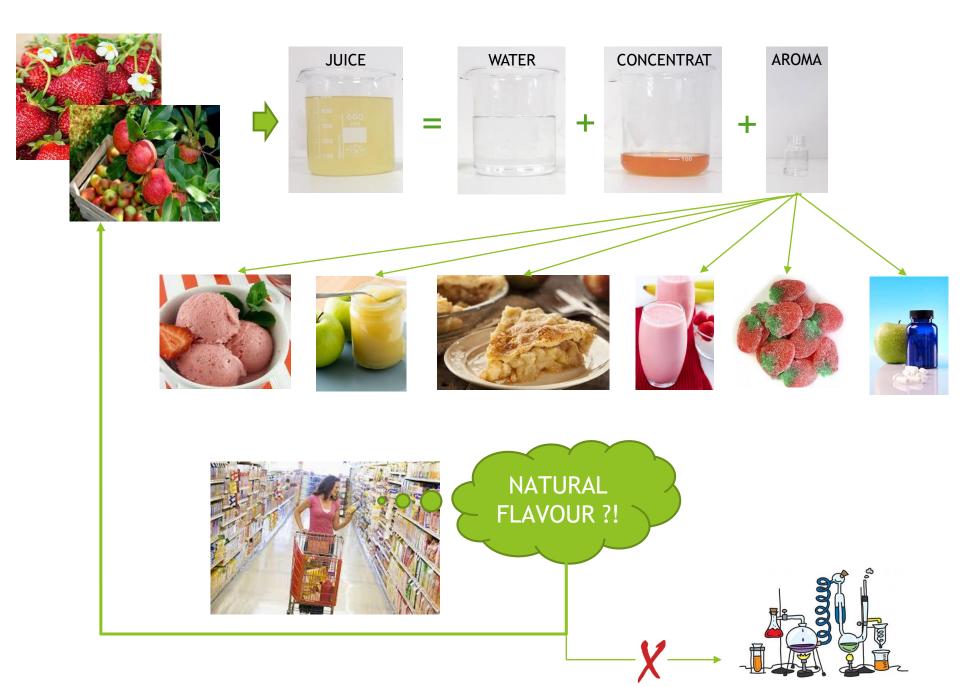
Authenticity assessment of fruit aroma compounds

Lidija Strojnik,

Department of Environmental Sciences, Jožef Stefan Institute

Jožef Stefan International Postgraduate School

Poster number: 8





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PRICE OF NATURAL VS SYNTHETIC AROMA!

NO ESTABLISHED ANALYTICAL METHOD!

-

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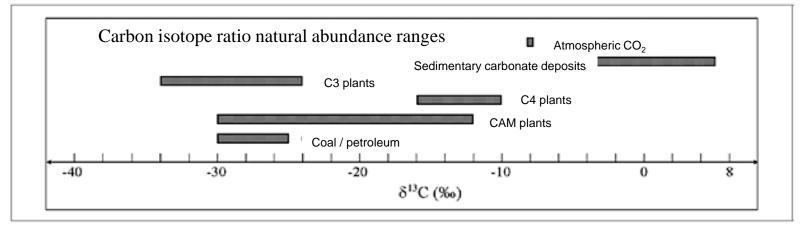


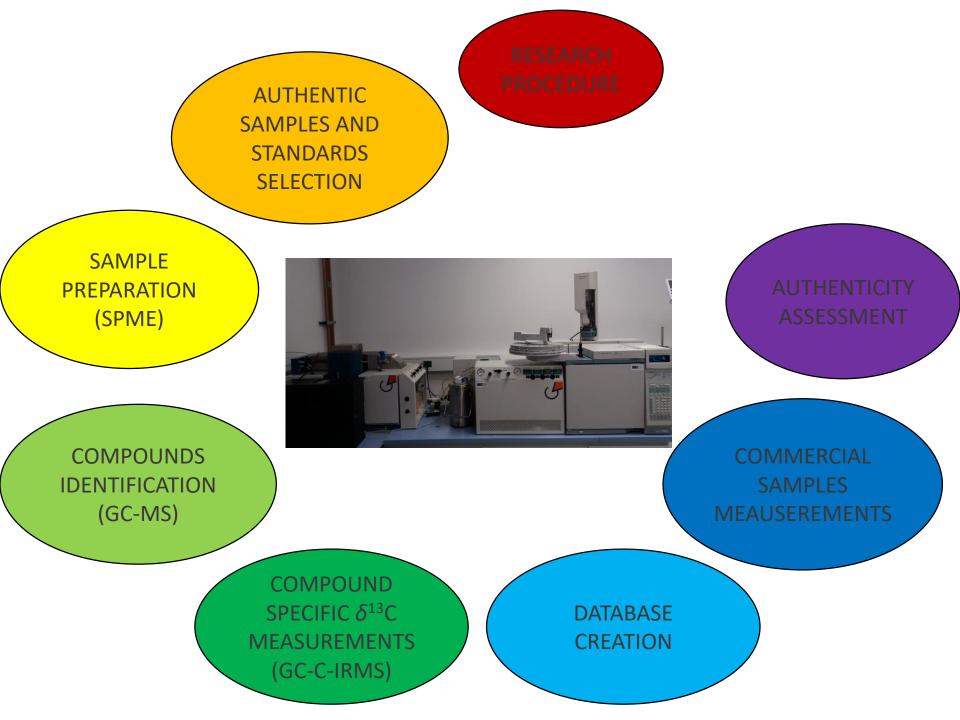
The use of discriminating analytical methodology

Carbon isotopes as tracers

comparing apples to "apples"

Gas Chromatography-Combustion-Isotope Ratio Mass Spectrometry (GC-C-IRMS)







Characterization of Slovenian apple and strawberry aromas for authenticity assessment using stable isotope approach

Strojnik Lidija^{1,2}, Stopar Matej³, Darinka Koron³, Zlatič Emil⁴, Kokalj Doris⁴, Naglič Gril Mateja⁵, Ženko Bernard⁶, Žnidaršič Martin⁶, Bohanec Marko⁶, Mileva Biljana⁶, Luštrek Mitja⁷, Gradišek Anton⁷, Potočnik Doris^{1,2}, Ogrinc Nives^{1,2}

Department of Environmental Science, John Statute, Unblanc, Science, 1000; "Scient International Fostgraduate School, Unblanc, Science, 2000; "Apricultural Institute of Science, Science, 2000; "Apricultural Institute of Science, Science, 2000; "April Science, Science, 2000; "April Science, Science, 2000; "Science, 2000; "April Science, 2000; "April Science, Science, 2000; "April Science, 2000; "April Science, Science, 2000; "April Science, 2000; Institute, Ljubljane, Slovenic, 2000

INTRODUCTION

Present work deals with the authenticity of raw materials such as natural flavourings. While natural aromas are becoming extensively used and natural raw materials are becoming more expensive, there is increasing pressure on prices and pronounced quality. Thus, many natural materials show the need for control of authenticity, as they are commonly being falsified in terms of dilution, mixing, or incorrect declaration of origin of natural resources. At the moment, gas chromatography isotope ratio mass spectrometry [GC-C-IRMS] is perhaps one of the most specific and sophisticated method for determining food authenticity.

METHODOLOGY

For authenticity assessment of aroma compounds several steps need to be taken, including optimization of extraction procedure; identification of aromatic components with GC-MSD; selection of working standard for 313C measurements; 313C measurements (component specific on GC-C-RMS); database creation from the obtained 313C values. The authenticity of the aroma compounds can then be verified by comparison of S¹³C of the analysed sample with the values from a created database. The established protocols and methods were also used in our study to investigate natural and commercially available apple and strawberry aroma distillates.

1) SAMPLES AND STANDARDS SELECTION





15 commercial distillates



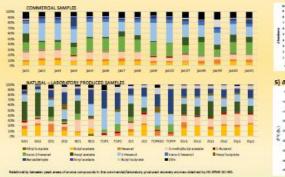
3) EXTRACTION PROCEDURE (HS-SPIME CONNECTED WITH GC-C-IRMS)



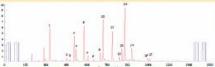
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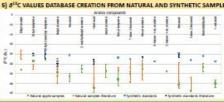


2) COMPOUND IDENTIFICATION



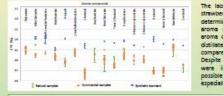
4) 5¹³C COMPONENT SPECIFIC MEASURMENTS ON GC-C-IRMS

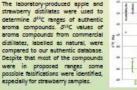




RESULTS

JUSC VALUES OF NATURAL AND COMMERCIAL APPLE DISTILLATES





T Return Lample A facture similar

5th C VALUES OF NATURAL AND COMMERCIAL STRAWBERRY DISTILLATES

CONCLUSIONS

Initial results show that GC-C-IRMS analysis of key volatile compounds is an appropriate tool for authenticity assessment of apple and strawberry distillates. Since many different compounds with different concentration are present in one sample, the selection of reference material and appropriate processing and interpretation of the results obtained is crucial. Finally, values of some aroma compounds in commercial samples indicate possible adulteration. To gain more confidence in the interpretation of measured values, an extensive database, which is under construction is required. We also noticed some deviation between natural apple and strawberry distillates for the same aroma compound. Differences may be in our future work better explain with the chemometrics and metabolomics approach.

Research is implemented in the framework of Smart Specialization Program: Food for Future and takes part of MASSTWIN (H2020, GA no. 692241) and ERA Chair ISO-FOOD (H2020, GA no. 621329) projects.

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Classification of stellar types based on RAVE stellar spectra morphology

llin Tolovski

International Postgraduate School Jožef Stefan

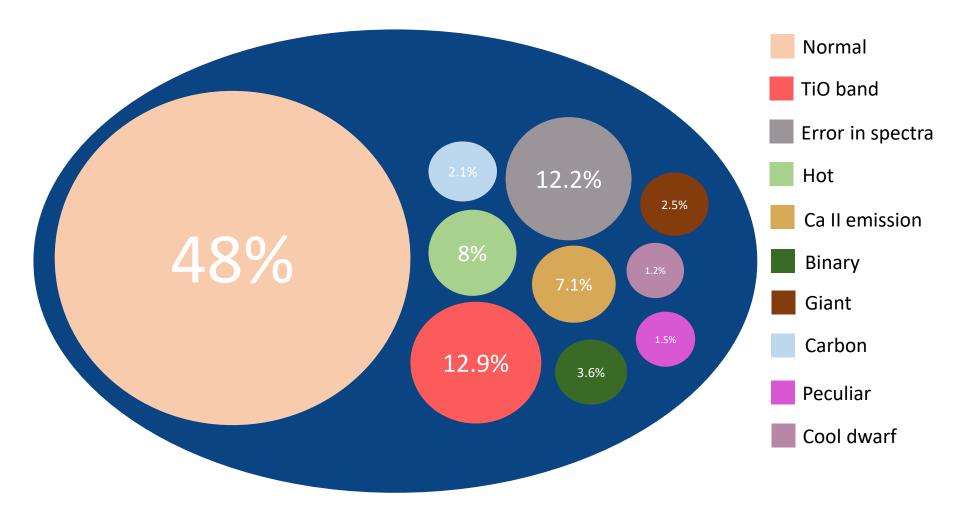
Department of Knowledge Technologies, Jožef Stefan Institute

Poster number: 19

Problem & data description

- RAVE (RAdial Velocity Experiment) Survey of the Milky Way
- Through these observations we study the history & morphology of the Milky Way
- Our dataset consists of stellar spectra described via:
 - 1522 (numeric) descriptive attributes
 - 1500 wavelengths
 - 19 linear integrals
 - 3 magnitudes of colors
 - 1 discrete target attribute
 - 4942 instances
- We used this data to predict the stellar type (12 classes)

The challenge



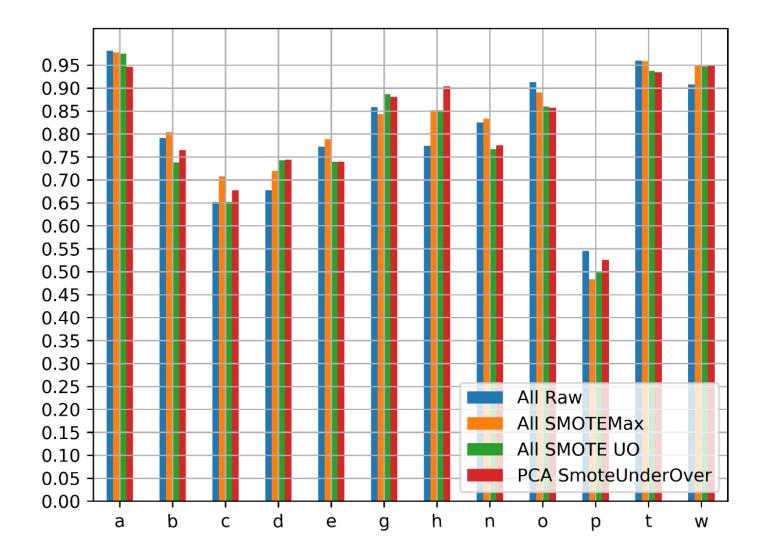
Methodologies

- Synthetic Minority Over-sampling Technique (SMOTE)
- Under-sampling
- Combination of under-sampling and SMOTE
- Dimensionality reduction (Principal Component Analysis)
- Data mining methods used for building predictive models:
 - Random Forest
 - Ensemble of Bagged Trees
- We use Matthews Correlation Coefficient (MCC) as the evaluation metric

 $MCC = \frac{TP*TN - FP*FN}{\sqrt{(TP+FP)(TP+FN)(TN+FP)(TN+FN)}}$

• Model evaluation through 10-fold cross-validation

Results & comparison of approaches





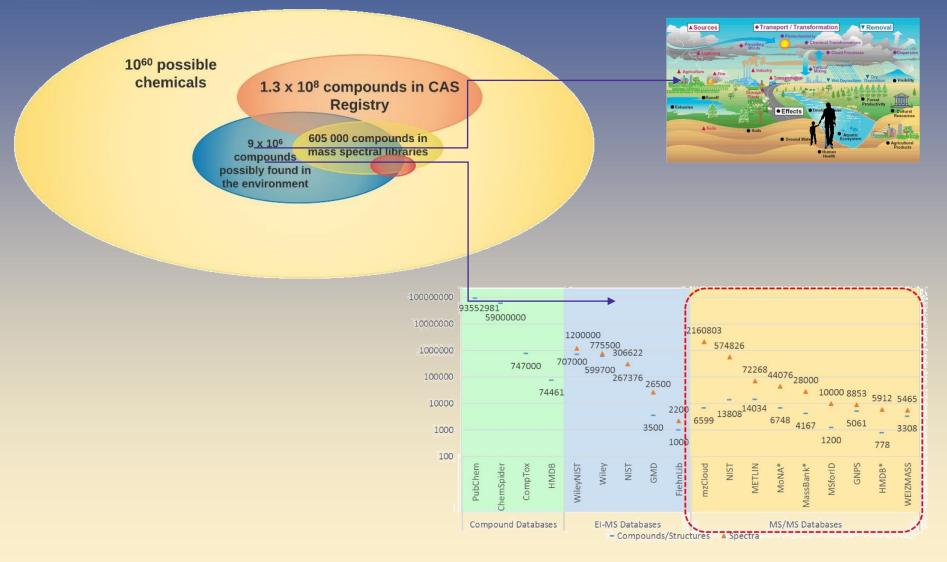
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Machine learning and non-target GC-EI-MS/MS environmental analysis – Do we have the perfect match?

Milka Ljoncheva PhD fellow, Department of Environmental Sciences, Jožef Stefan Institute Poster number : 38

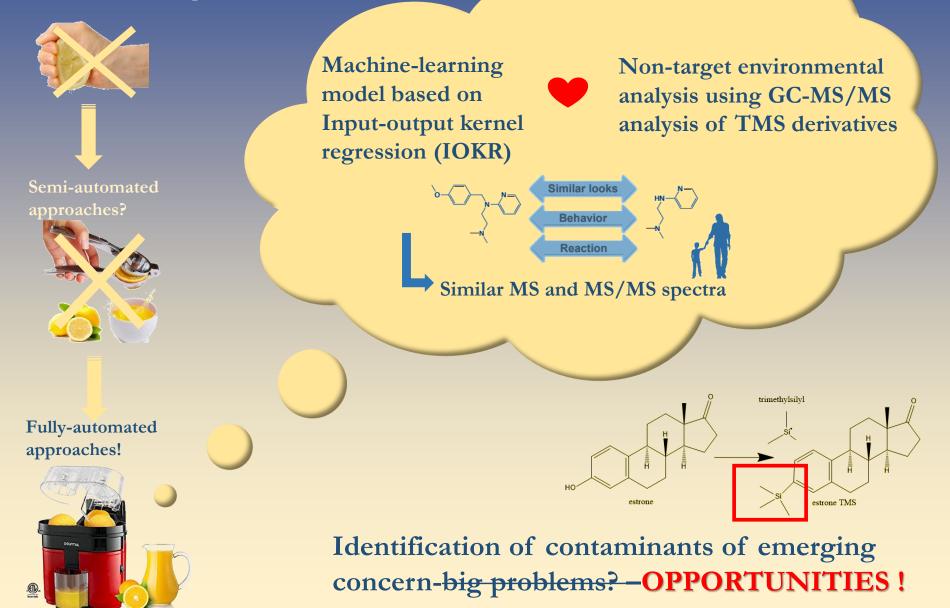
Identification of contaminants of emerging concern (CECs)- big problems?



How to annotate the unknowns?

How to squeeze the lemon properly?

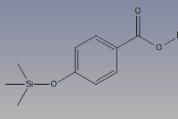
Manual MS/MS interpretation?



Generation of test dataset

CECs of interest: 110 compounds, 20 compounds analyzed 60 EI-MS and 40 EI-MS/MS spectra generated

Parabens

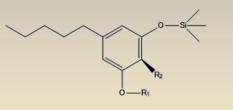


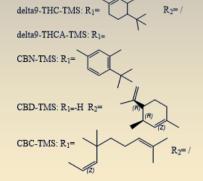
methylparaben TMS: R= -CH3 ethylparaben TMS: R= -CH2-CH3 propylparaben TMS: R= -CH2-CH2-CH3 isopropylparaben TMS: R= -CH₂(CH₃)CH₃ butylparaben TMS: R= -CH2CH2CH2CH3 benzylparaben TMS: R= -CH2-Ph

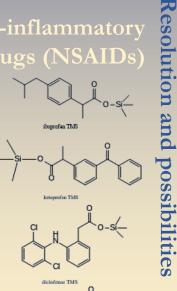


Non-steroidal anti-inflammatory

Natural cannabinoids







drugs (NSAIDs)

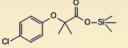
Estrogen hormones

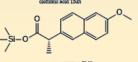
estrone TMS: R1=-C=O R2=-

estriol TMS: R1= -OH R2= -OH

17-beta-estradiol TMS: R1=-OH R2=

ethinylestradiol TMS: R1=-OH(C = C) R2=









 MS^1 , MS^2



GC-EI-Ion Trap MS¹, MS²....MSⁿ

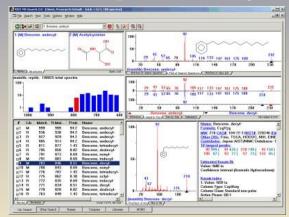


Generation of training dataset

Literature (2014-2018), prediction systems, library of transformations

In-house database of most important CECs (~6300 compounds)

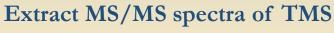
• NIST Mass spectral library 2017

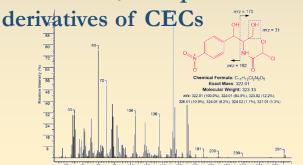


Use the IOKR model on real non-target environmental analysis

Mission complete !

Evaluate and validate CECs identification performance of the developed method







Thank you for your attention !

For more info, visit poster no.38

Science never solves a problem without creating ten more.

-George Bernard Shaw

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Alternative method for advanced tissue healing using piezoelectric materials

Lea Udovč,

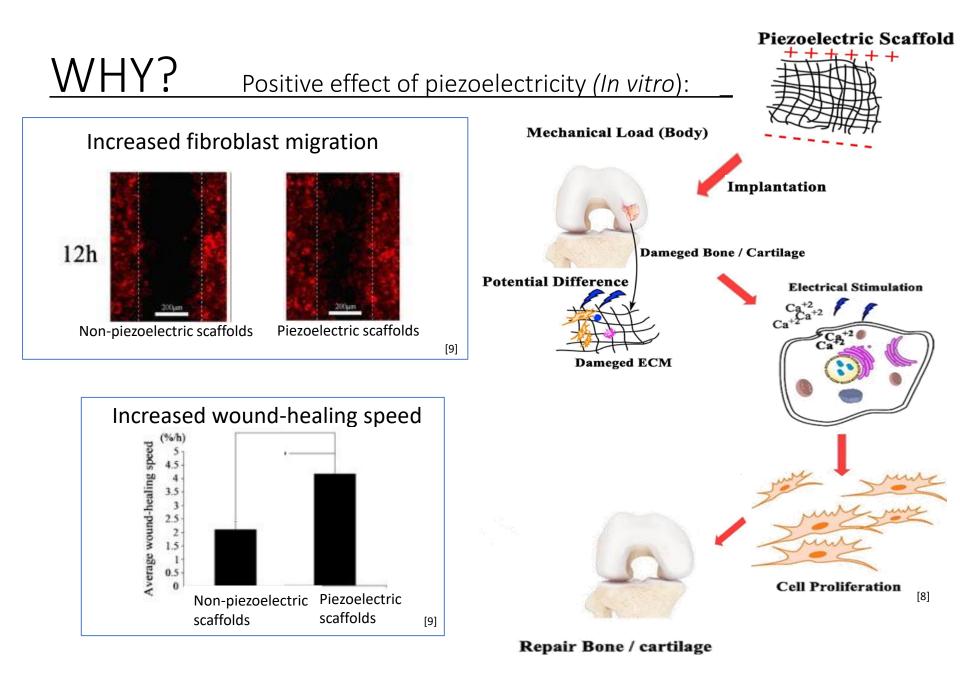
Advanced Materials Department K9, Jožef Stefan Institute, and Jožef Stefan International Postgraduate School

Poster number: 27

WHAT?

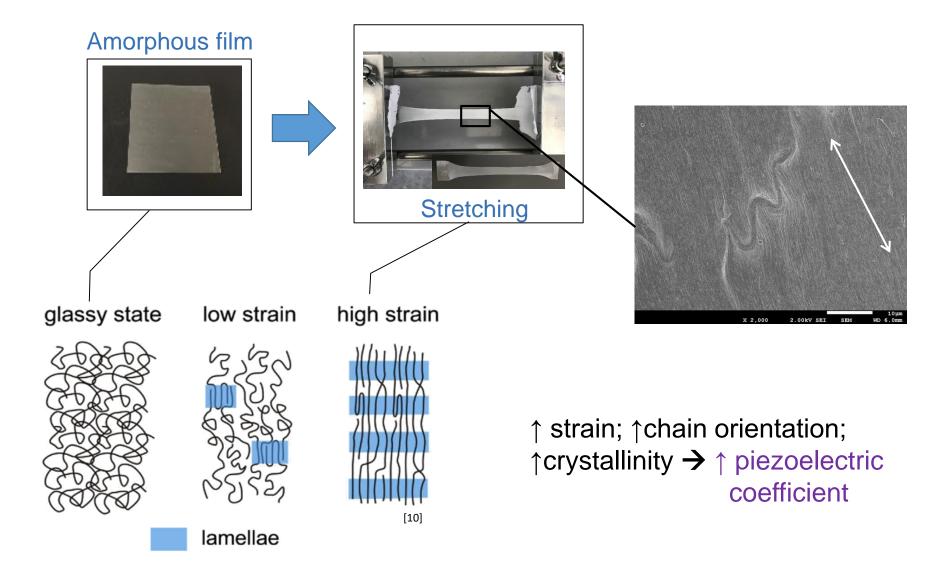


[1] https://www.researchgate.net/figure/Molecular-structure-of-PLA_fig1_261102190; [2] http://www.piezofilms.com/; [3] http://dwitnews.com/after-a-leg-break/; [4] https://www.nobelbiocare.com/au/en/education/dental-implantology-courses/implant-placement-courses.html; [5] https://www.dreamstime.com/stock-illustration-calf-muscle-tear-medical-illustration-symptoms-image68893791; [6] http://www.europeanmedical.info/tissue-engineering/twodimensional-clinical-tissue-engineering.html; [7] http://slideplayer.com/slide/10750224/



[8] N. More, G. Kapusetti, Medical Hypotheses, 2017, 108, 10-16; [9] H. F. Guo, Z. S. Li, S. W. Dong, W. J. Chen, L. Deng, Y. F. Ying, Colloids and Surfaces B: Biointerfaces, 2012, 96, 29-36

HOW? Strain induced crystallization of PLA



[10] Y. Yin, X. Zhang, Y. Song, S. de Vos, R. Wang, C. A. P. Josiasse, G. Liu, D. Wang, Polymer., 2015, 65, 223–232.

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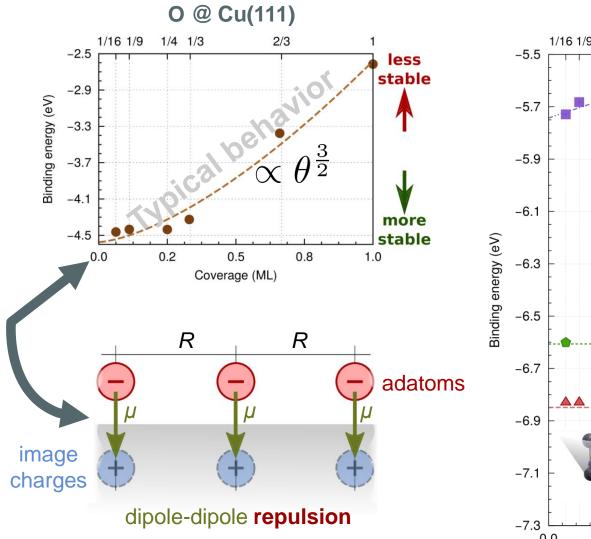
Opposite charges attract and like charges repel. Do they always?

Matic Poberžnik,

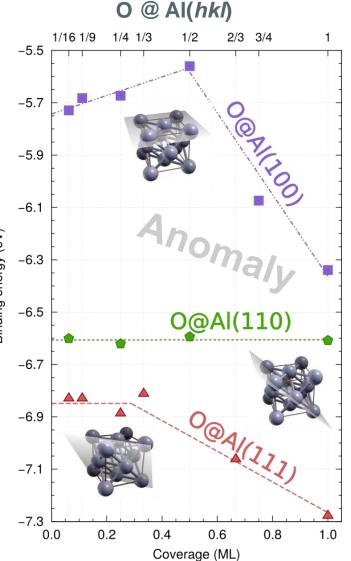
Jožef Stefan Institute

Poster number: 03

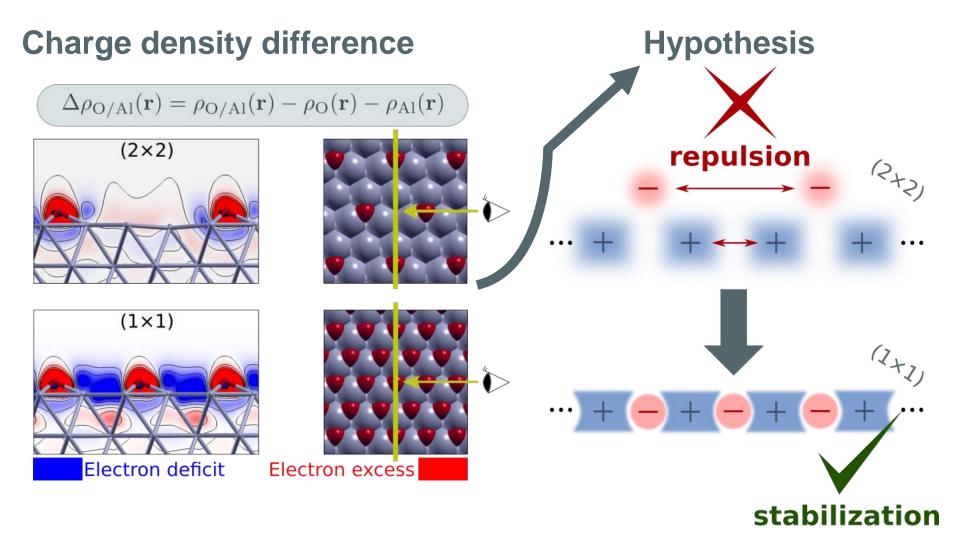
PROBLEM



M. Poberžnik, A. Kokalj, J. Phys. Chem. C 120, 45, 2016.

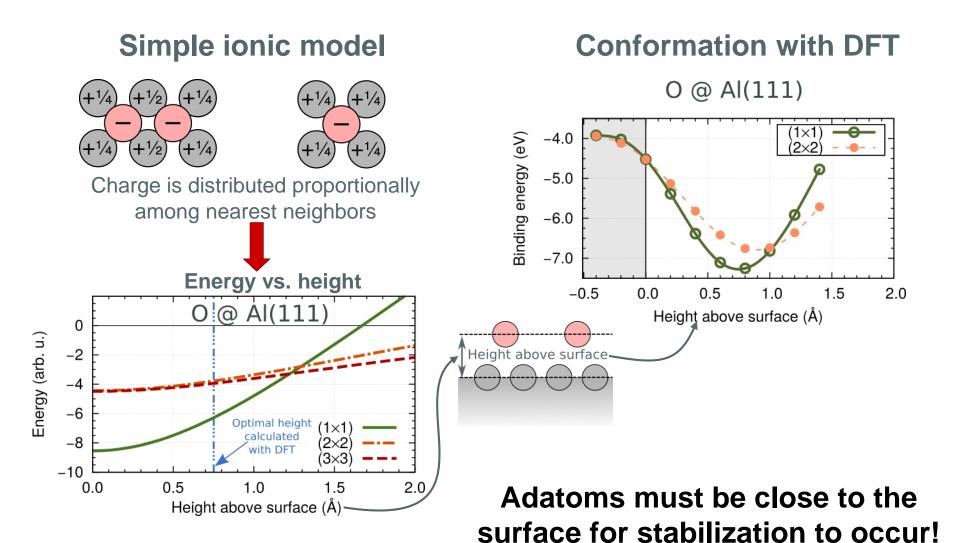


ANALYSIS



M. Poberžnik, A. Kokalj, J. Phys. Chem. C 120, 45, 2016.

EXPLANATION



M. Poberžnik, A. Kokalj, J. Phys. Chem. C 120, 45, 2016.

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Blood Pressure Prediction Using Data Mining Algorithms

Ana Kostovska,

Department of Knowledge Technologies, Jožef Stefan Institute, Ljubljana, Slovenia

Jožef Stefan International Postgraduate School, Ljubljana, Slovenia

Poster number: 2

Problem description

- Hypotension (low blood pressure) and especially hypertension (high blood pressure) are heart diseases of global health concern.
- Chronic exposure to these medical conditions can gradually damage the entire body.
- To improve the treatment, it's crucially important to monitor the blood pressure on a regular basis.
- We develop models that give an approximate estimate of the blood pressure in real time using personal data and data collected from sensors.





Data description & evaluation metric

- The dataset consists of:
 - 1429 data points
 - 18 descriptive features
 - 3 target features: systolic, diastolic & pulse
 - Measurements from 96 different patients
 - Multiple measurements per patient
- For evaluating the performance of the models, we measure the Mean Absolute Error (MAE)
- We use the leave-one-patient-out validation approach





Methodology and results

Data mining methods used for building predictive models:

- Linear Regression (LR)
- Bagging of Regression Trees (BRT)
- Gradient Boosting of Regression Trees (GBRT)
- Bagging of Model Trees (BMT)
- Bagging of Random Subspaces with Model Trees (BRSMT)

	Systolic pressure	Diastolic pressure	Pulse pressure	Systolic and diastolic pressure	Systolic and pulse pressure
ZeroR	14.9524	9.3724	13.2530		
LR	11.6538	8.5061	11.3592		
BRT	11.5864	9.1573	11.2947	11.3963	11.2832
GBRT	10.6130	8.8098	10.9169		
вмт	11.3998	9.1103	11.2965		
BRSMT	10.9649	8.855142	11.0889		





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Topological defects in smectic ordering.

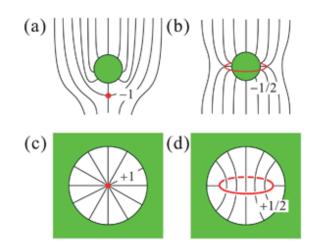
Apparao Gudimalla,

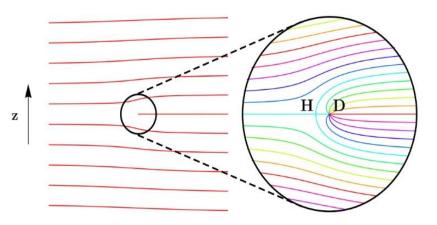
Jozef Stefan International Postgraduate School

Poster number: 30

Introduction

- Topological defects (TDs) are ubiquitous in nature, which is commonly introduced bulk ordering properties
- An isolated TD could not be destroyed if the field in not melted due to the topological reasons
- TDs are generated by symmetry breaking mechanism (systems with broken symmetries are described by non-vanishing order parameter).
- TDs are experimentally accessible, so that different liquid crystal phases are an ideal choice





Modeling of dislocations in smectic A liquid crystals

 $f = f_c + f_e^{(n)} + f_e^{(s)}$ $f_e^{(s)}$ $= \alpha (T - T_c) |\varphi|^2 + \beta |\varphi|^4 + C_{\parallel} |(iq_0 \vec{n} - \nabla)\varphi|^2$

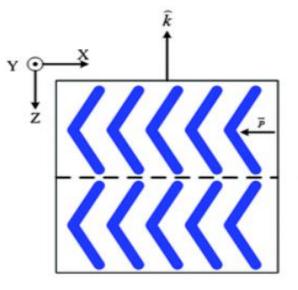
$$f = \propto_0 \left(T - T_c \right) |\varphi|^2 + \beta |\varphi|^4 + \frac{\hbar^2}{4m} \left| \left(\nabla - \frac{2ie}{\hbar C} \vec{A} \right) \varphi \right|^2 + \frac{\left| \nabla \times \vec{A} \right|^2}{8\pi \mu_0}$$

 $+ C_{\perp} |(\vec{n} \times \nabla) \varphi|^2$

Introducing the edge dislocations

- The system avoided strong local bend distortion by melting
- Another possible scenario is that lattice of edge dislocation is introduced
- Ratio of smectic-A phase

$$\delta = \lambda/\xi$$



$$\lambda = \sqrt{\frac{K}{2C_{\perp} \eta^2 q_0^2}}$$

$$\xi = \sqrt{\frac{2C_{\perp}}{\partial^2 f_c / \partial \eta^2}}$$

Conclusion

- Similar free energy expression for the smectic and superconducting ordering suggest that also another solution to the problem
- Smectic-A phase characterized by $\lambda/\xi > 1/\sqrt{2}$ smectic bend imposed frustration could be resolved by a lattice edge dislocations
- The present problem that I am going to explore theoretically and experimentally

Thank you

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Hybrid sol-gel coatings for corrosion protection of aluminum alloy AA7075

Urša Tiringer

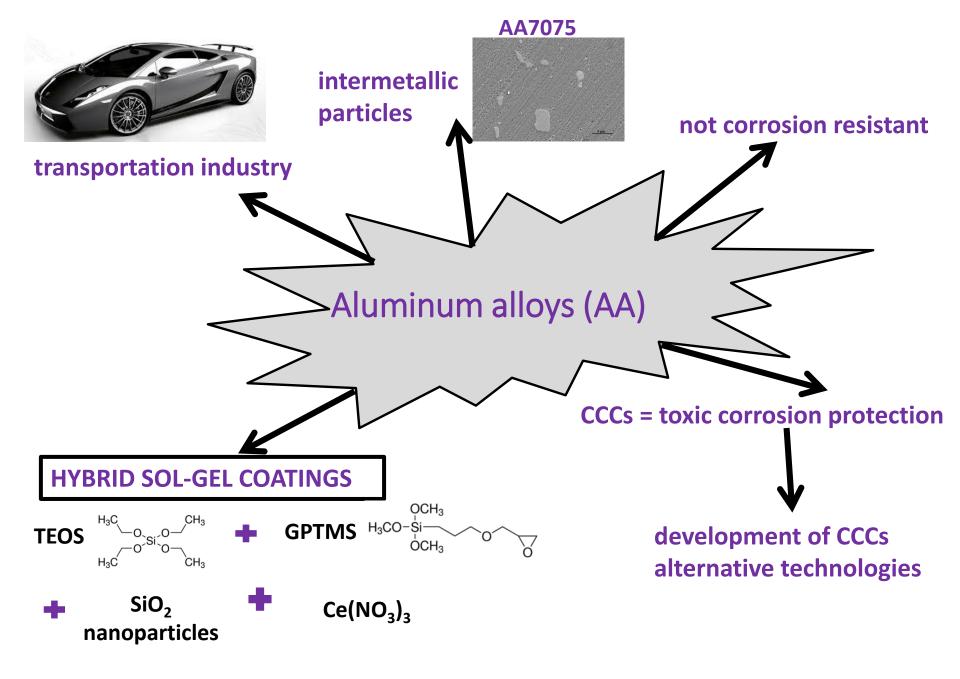
Jožef stefan institute, Department of Physical and Organic Chemistry,

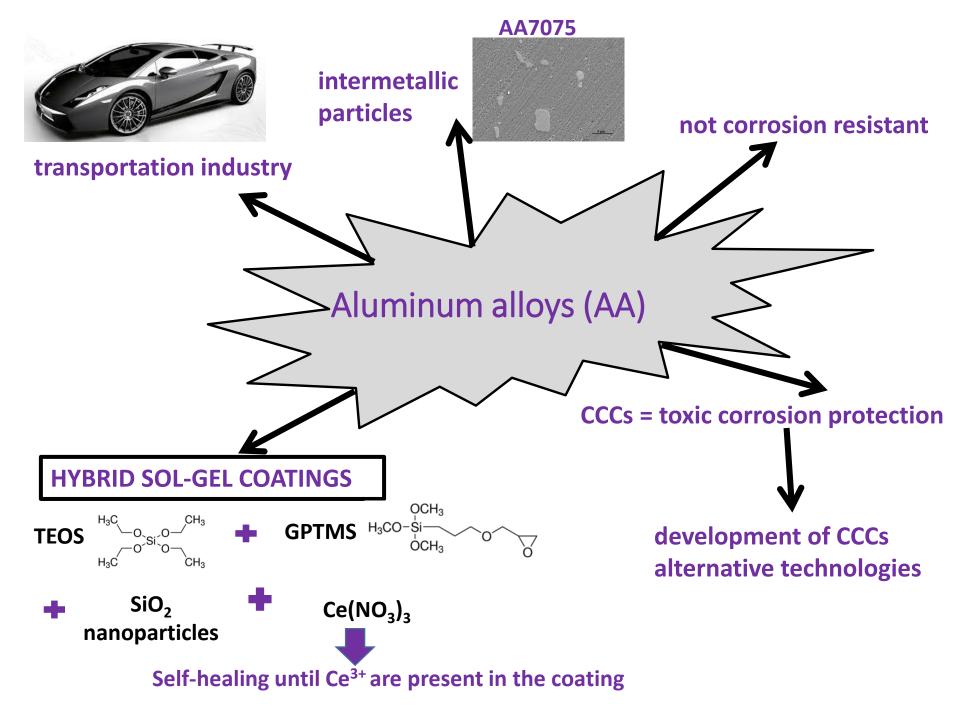
Ljubljana, Slovenia

Jožef Stefan International Postgraduate School, Nanoscience and Nanotechnology

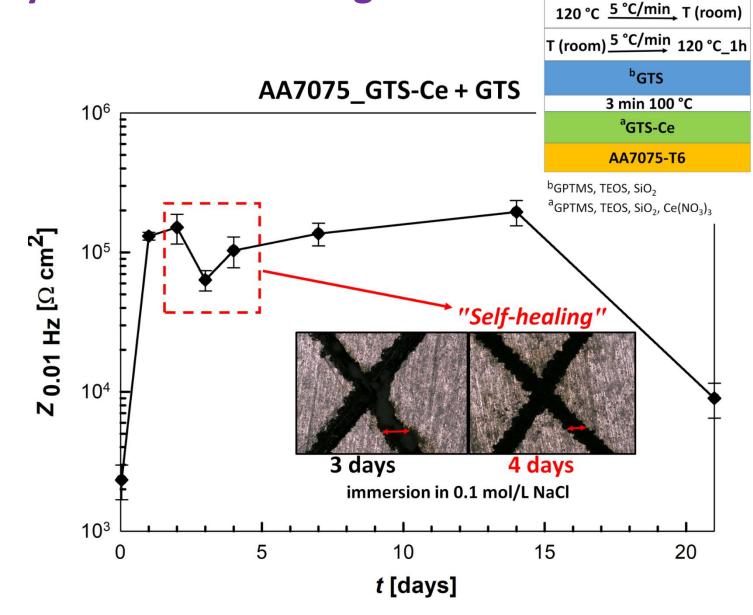
Ljubljana, Slovenia

Poster number: 24

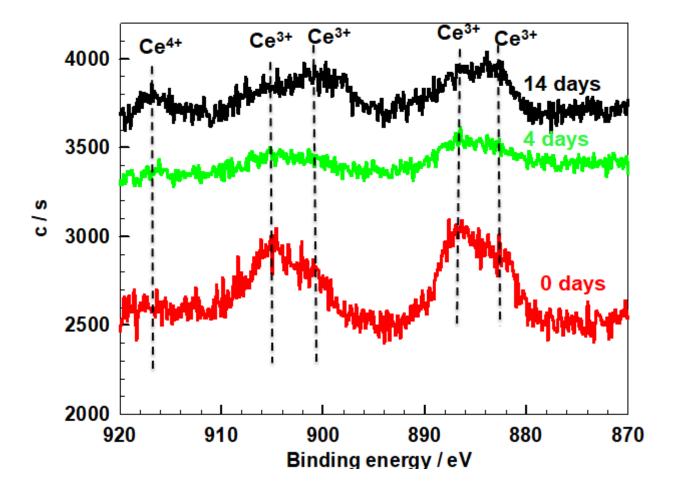




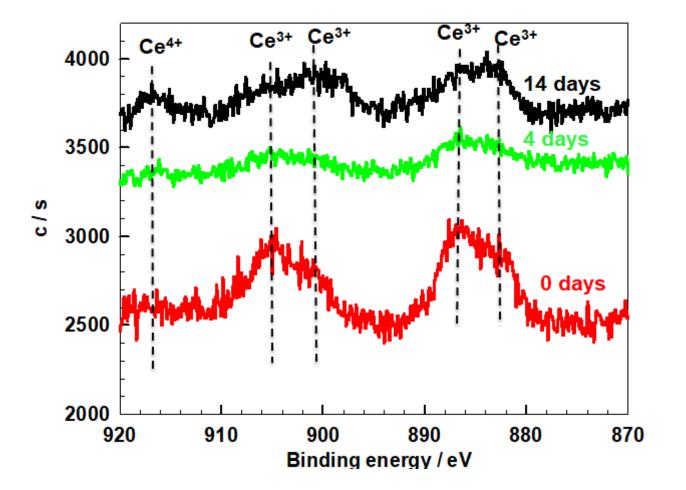
Study of the self-healing effect



High resolution spectra of Ce 3d on scribe of GTS-Ce + GTS immersed in 0.1 M NaCl for different times



High resolution spectra of Ce 3d on scribe of GTS-Ce + GTS immersed in 0.1 M NaCl for different times



Self-healing is efficient after 14 days of immersion!

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A Semi – Automatic Approach for Borrowing Missing Nutrient Values in Food Composition Databases

Gordana Ispirova

Computer Systems Department, Jožef Stefan Institute, Ljubljana Slovenia

Jožef Stefan International Postgraduate School, Ljubljana, Slovenia

Poster number: 34

Food Composition Databases (FCDBs)

Pro:

• very useful tool

Con:

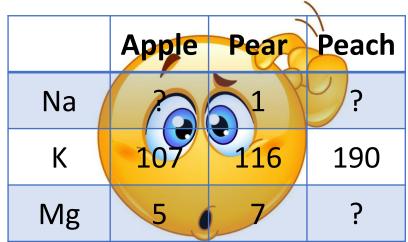
• a lot of limitations

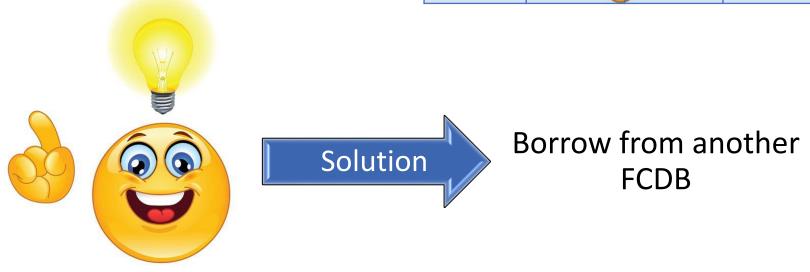
Nutrient	Unit	1 Value Per100 g	1 cup, quartered or chopped 125g	1 cup slices 109g	1 large (3-1/4" dia) 223g	1 medium (3" dia) 182g	1 small (2-3/4" dia) 149g	1 extra small (2-1/2" dia) 101g	1 NLEA serving 242g
Proximates									
Water	g	85.56	106.95	93.26	190.80	155.72	127.48	86.42	207.06
Energy	kcal	52	65	57	116	95	77	53	126
Protein	g	0.26	0.33	0.28	0.58	0.47	0.39	0.26	0.63
Total lipid (fat)	g	0.17	0.21	0.19	0.38	0.31	0.25	0.17	0.41
Carbohydrate, by difference	g	13.81	17.26	15.05	30.80	25.13	20.58	13.95	33.42
Fiber, total dietary	g	2.4	3.0	2.6	5.4	4.4	3.6	2.4	5.8
Sugars, total	g	10.39	12.99	11.33	23.17	18.91	15.48	10.49	25.14
Minerals									
Calcium, Ca	mg	6	8	7	13	11	9	6	15
Iron, Fe	mg	0.12	0.15	0.13	0.27	0.22	0.18	0.12	0.29
Magnesium, Mg	mg	5	6	5	11	9	7	5	12
Phosphorus, P	mg	11	14	12	25	20	16	11	27

Scenario: Using a FCDB Problem: Missing values

	Apple	Pear	Peach
Na	?	1	?
К	107	116	190
Mg	5	7	?

Scenario: Using a FCDB Problem: Missing values





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Scenario: Choosing a FCDB for borrowing Problem: PROBLEMS!

The FCDB for borrowing must:

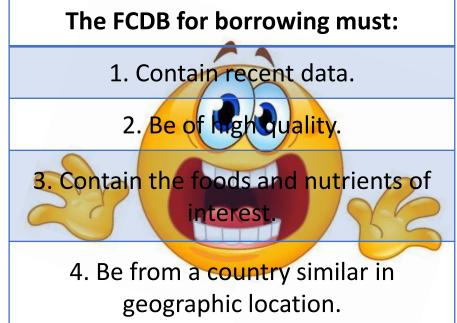
1. Contain recent data.

2. Be of high quality.

3. Contain the foods and nutrients of interest.

4. Be from a country similar in geographic location.

Scenario: Choosing a FCDB for borrowing Problem: PROBLEMS!



Solution?!

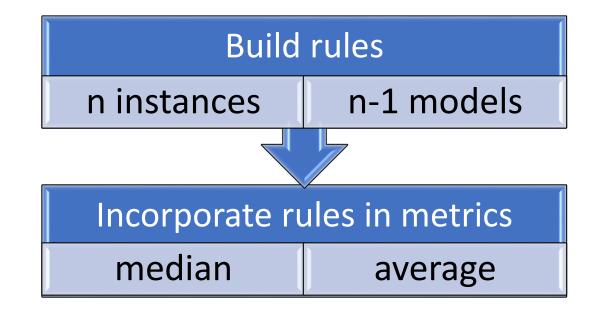
Gordana Ispirova, Poster #34

Method

Data:

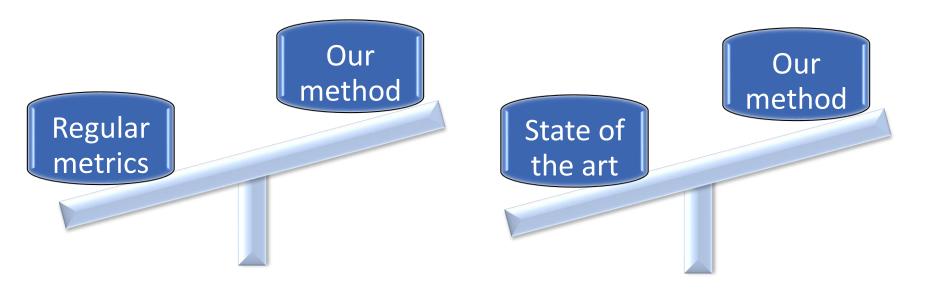
	Country ₁	Country ₂	 Country _m
Nutrient ₁	Value ₁₁	Value ₁₂	 Value _{1m}
:	÷	÷	 ÷
Nutrient _n	Value _{n1}	Value _{n2}	 Value _{nm}

Methodology:



Results

- Leave-one-out-cross-validation
 - 14 nutrients in **Beef Fillet** from FCDBs of 10 countries
- Evaluation



THANK YOU FOR YOUR ATTENTION!



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Highly Efficient Carbon Nanostructures:- Exciting Solution For The Energy Storage Devices

Neelakandan Marath Santhosh

Jožef Stefan International Postgraduate School (IPS),

Ljubljana, Slovenia

Poster number: 04



CARBON NANOSTRUCTURES

Our Suggestion:- 2D Carbon Structures

Carbon containing hydrogels- resorcinolformaldehyde, cellulose hydrogel, phenolformaldehyde Ar, H₂ gas

Plasma treatment

Elevating temperature, dissociation into different radicals, etching of amorphous phase

Carbon nanowall/ nanostructures with uniform morphology and inter layer spacing

Advantages of Our Technique

- One-step low time synthesis technique
- Possibility to control the morphology
- Chances for the various carbon nanostructure (carbon

nanowall, carbon nanosheets, etc.)

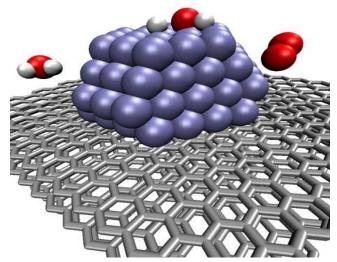
- In-situ plasma assisted surface modification
- Easier and safer technique

Applications

Energy storage devices (electrodes)







SuperLithiumcapacitorsBattery

Catalyst supporter for fuel cells

- Recharge an electronic device (smart phone, laptops, cameras) within minutes ?
- Requires advanced material for short-term power boosting in space applications ?
- Making an eco-friendly fuel cells and replace the toxic lead-acid batteries.

Jhanks For Your Kind Attention

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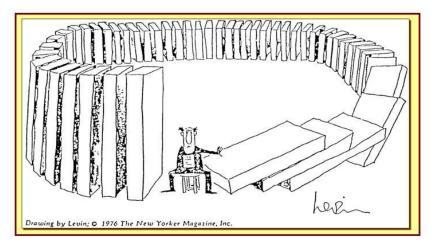
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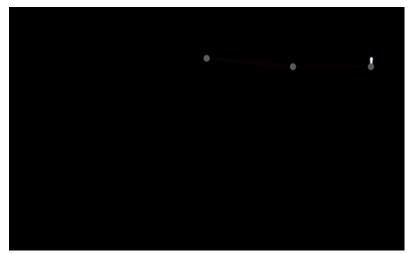
Identification of a Nonlinear Dynamical Benchmark System using Process-Based Modeling

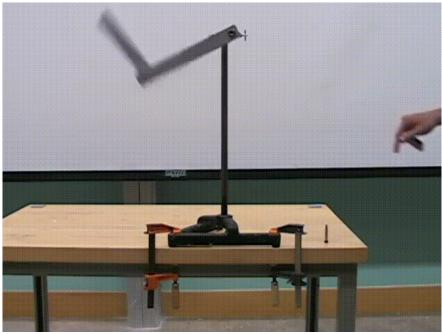
Gjorgi Peev, Department of Knowledge Technologies, Jožef Stefan Institute, Ljubljana, Slovenia Poster number: 37

Dynamical systems

Dynamic Complexity is All Around Us

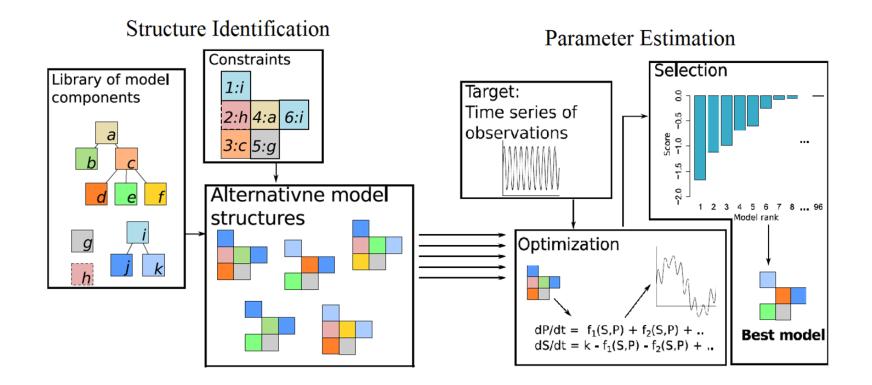


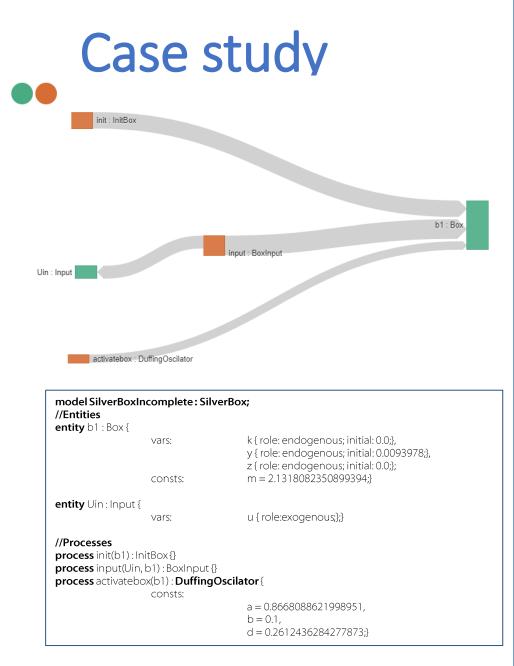




Gjorgi Peev, Poster #37

Process-Based Modeling





library SilverBox;							
// Entity templates							
template entity Box { template entity Input {		vars: k {aggregation:sum}, y {aggregation:sum}, z {aggregation:sum}; consts: m {range: <0.1,100>};} vars: u {aggregation:sum};}					
// Process templates		a (aggi agation barrij)					
template process InitBox (b: Box) {							
template process initibox (b. box) {		equations:	td(b.y) = b.z;}				
template process BoxInput(v: Input, b: Box		<pre> { equations: </pre>	td(b.z) = (v.u) / b.m;}				
template process Bo	oxAction (b: Box) {}						
template process DuffingAndSimple : BoxAction { consts:							
	equations:	a {range: <0.1,100>}, b {range: <0.1,100>};					
	equations.	b.k = a + b * pow(b.y,2);					
template process HarmonicAndUniversal : BoxAction {							
	consts: equations:	ksi {range: <0.1,100>};					
		b.k=0;}					
template process DuffingOscilator: DuffingAndSimple {							
	consts: equations:	d {range: <0.1,100>};					
		td(b.z) = (- b.k * b.y - d* b.z) / b.m;}					
template process Si	mpleOscilator: Duffing equations:	gAndSimple { td(b.z) = (- b.k * b.y) / b.m;}					
template process HarmonicOscilator: HarmonicAndUniversal{							
consts:		omega {range: <0.1,100>};					
	equations: td(b.z) = (-ksi*omega*	*b.z-pow(omega,2)*b.y);}					
template process UniversialOscilator: HarmonicAndUniversal {							
	consts: equations:	q {range: <0.1,100>};					
		td(b.z) = (-ksi*b.z - q);}					

Gjorgi Peev, Poster #37

Thank you for your attention

• For more information, visit poster #37

#GrazieRagazzi

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coffee break