Abstract
Cover letter

Igor Pašti

Istraživanje

- **Identifikacija tematike/Pretraga literature**
- Postavka eksperimenta
- Izrada eksperimenta
- Analiza i diskusija rezultata
- Priprema publikacije
- Proces publikovanja

Identifikacija teme – predmeta istraživanja

Zašto?

Da li postoji veza između broja pomorandži u prodavnici sa ukupnim brojem proizvoda bez glutena?

vs.

Istraživanje

- Identifikacija tematike/Pretraga literature
- **Postavka eksperimenta**
- Izrada eksperimenta
- Analiza i diskusija rezultata
- Priprema publikacije
- Proces publikovanja

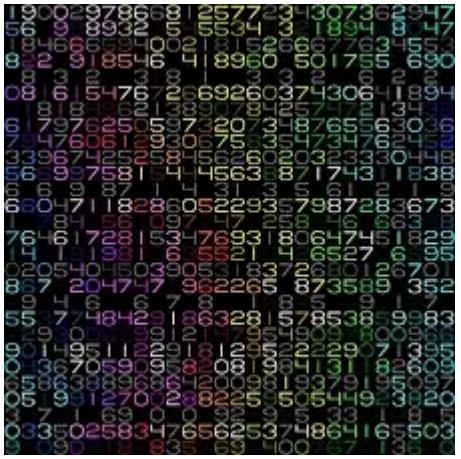
Postavka eksperimenta

- Analiza broja prodavnica
- Prebrojavanje proizvoda
- Prikupljanje podataka
- Izbor statističke metode
- ...

Istraživanje

- Identifikacija tematike/Pretraga literature
- Postavka eksperimenta
- **Izrada eksperimenta**
- Analiza i diskusija rezultata
- Priprema publikacije
- Proces publikovanja

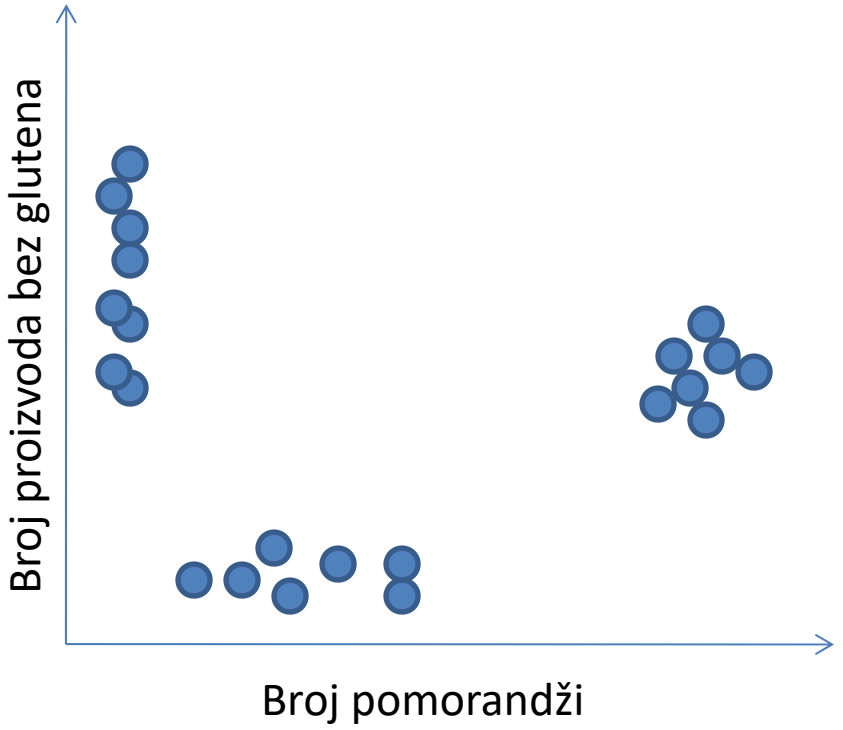
Izrada eksperimenta



Istraživanje

- Identifikacija tematike/Pretraga literature
- Postavka eksperimenta
- Izrada eksperimenta
- **Analiza i diskusija rezultata**
- Priprema publikacije
- Proces publikovanja

Analiza i diskusija rezultata



Zaključci:

1. Ima li korelacije
2. Ima li grupisanja
3. Može li se povezati sa tipom prodavnice

Analiza i diskusija rezultata

Broj proizvoda bez glutena

Broj pomorandži

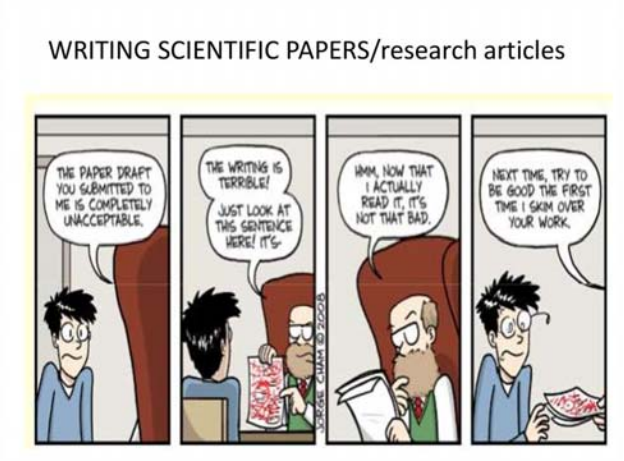
Glavni zaključci su...

Istraživanje

- Identifikacija tematike/Pretraga literature
- Postavka eksperimenta
- Izrada eksperimenta
- Analiza i diskusija rezultata
- **Priprema publikacije**
- Proces publikovanja

Priprema publikacije

- Odabir časopisa (kriterijumi)
- Priprema manuscripta
- Korekcije, korekcije, korekcije
- Još korekcija...
- Slanje manuscripta
- Proces recenzije / revizije
- Čestitamo, objavili ste rad



Struktura članka

- Uvod
- Materijal / metode / experimental
- Rezultati
- Diskusija
- Zaključak
- Literatura



- Identifikacija tematike/Pretraga literature
- Postavka eksperimenta
- Izrada eksperimenta
- Analiza i diskusija rezultata

Struktura članka

ABSTRAKT

- Uvod
- Materijal / metode / experimental
- Rezultati
- Diskusija
- Zaključak
- Literatura

Abstrakt

- An abstract is a brief summary of a research article, thesis, review, conference proceeding, or any in-depth analysis of a particular subject and is often used to help the reader quickly ascertain the paper's purpose.

- Gary Blake and Robert W. Bly, The Elements of Technical Writing, pg. 117. New York: Macmillan Publishers, 1993. ISBN 0020130856

Indian J Psychiatry. 2011 Apr-Jun; 53(2): 172–175.
doi: 10.4103/0019-5545.82558
PMCID: PMC3136027
PMID: 21772657

How to write a good abstract for a scientific paper or conference presentation

Chittaranjan Andrade

‣ Author information ‣ Copyright and License information Disclaimer

Abstract

Go to:

Abstracts of scientific papers are sometimes poorly written, often lack important information, and occasionally convey a biased picture. This paper provides detailed suggestions, with examples, for writing the background, methods, results, and conclusions sections of a good abstract. The primary target of this paper is the young researcher; however, authors with all levels of experience may find useful ideas in the paper.

Keywords: Abstract, preparing a manuscript, writing skills

INTRODUCTION

Go to:

- “Only a reader with a very specific interest in the subject of the paper, and a need to understand it thoroughly, will read the entire paper.”

- “Thus, for the vast majority of readers, the paper does not exist beyond its abstract.”

Indian J Psychiatry. 2011 Apr-Jun; 53(2): 172–175.

Tipovi abstrakta

- Descriptive
- Informative
- Structured
- Semi-structured
- Non structured

J Indian Prosthodont Soc. 2013 Sep; 13(3): 382–383

Tipovi abstrakta

- Descriptive

This type of abstract is usually very short (50–100 words). Most descriptive abstracts have certain key parts in common. They are:

□ Background

□ Purpose

□ Particular interest/focus of paper

□ Overview of contents (not always included)

J Indian Prosthodont Soc. 2013 Sep; 13(3): 382–383

Tipovi abstrakta

- Informative

From these abstracts, you must get the essence of what your report is about, usually in about 200 words. Most informative abstracts also have key parts in common. Each of these parts might consist of 1–2 sentences. The parts include:

□ Background

□ Aim or purpose of research

□ Method used

□ Findings/results

□ Conclusion

J Indian Prosthodont Soc. 2013 Sep; 13(3): 382–383

Tipovi abstrakta

- Structured

A structured abstract has a *paragraph for each section: Introduction, Materials and Methods, Results, and Conclusion* (it may even include paragraphs for the objectives or other sections).

J Indian Prosthodont Soc. 2013 Sep; 13(3): 382–383

Tipovi abstrakta

- Semi-structured

A semi-structured abstract *is written in only one paragraph, where each sentence corresponds to a section*. All the sections of the article are present as in the structured abstract

J Indian Prosthodont Soc. 2013 Sep; 13(3): 382–383

Tipovi abstrakta

- Non structured

When the abstract *does not present divisions between each section*, and it may not even present any of them, it is a non-structured abstract. The sentences are included in a sole paragraph. This type of presentation is *ideal for descriptive abstracts*

J Indian Prosthodont Soc. 2013 Sep; 13(3): 382–383

Planiranje abstrakta

Introduction—what is the topic?

Statement of purpose?

Summarize why have other studies not tackled similar research questions?

How has the research question been tackled?

How was the research done?

What is the key impact of the research?

J Indian Prosthodont Soc. 2013 Sep; 13(3): 382–383

Nekoliko primera (ACS author guide)

One or two sentences providing background on the problem.

Two or three sentences summarizing the methodology and results.

A concluding sentence highlighting the significance of the study.

Nitrogen oxides, including nitrogen dioxide and nitric acid, react with mineral dust particles in the atmosphere to yield adsorbed nitrate. Although nitrate ion is a well-known chromophore in natural waters, little is known about the surface photochemistry of nitrate adsorbed on mineral particles. In this study, nitrate adsorbed on aluminum oxide, a model system for mineral dust aerosol, is irradiated with broadband light ($\lambda > 300$ nm) as a function of relative humidity (RH) in the presence of molecular oxygen. Upon irradiation, the nitrate ion readily undergoes photolysis to yield nitrogen-containing gas-phase products including NO_2, NO, and N_2O, with NO being the major product. The relative ratio and product yields of these gas-phase products change with RH, with N_2O production being highest at the higher relative humidities. Furthermore, an efficient dark reaction readily converts the major NO product into NO_2 during post-irradiation. Photochemical processes on mineral dust aerosol surfaces have the potential to impact the chemical balance of the atmosphere, yet little is known about these processes. In this study, the impact that adsorbed nitrate photochemistry may have on the renoxification of the atmosphere is discussed. (*J. Phys. Chem. A* **2009,** *113,* 7818–7825).

Nekoliko primera (ACS author guide)

Polymer-fullerene bilayer heterostructures are suited to study excitonic processes in conjugated polymers. Excitons are efficiently quenched at the polymer-fullerene interface, whereas the polymer-vacuum interface is often considered as an exciton-reflecting interface. Here, we report about efficient exciton quenching close to the polymer-vacuum interface of spin-coated MDMO-PPV (poly[2-methoxy-5-(2′-ethyl-hexyloxy)-*p*-phenylenevinylene]) films. The quenching efficiency is estimated to be as high as that of the polymer-fullerene interface. This efficient quenching is consistent with enhanced intermolecular interactions close to the polymer-vacuum interface due to the formation of a "skin layer" during the spin-coating procedure. In the skin layer, the polymer density is higher; that is, the intermolecular distances are shorter than in the rest of the film. The effect of exciton quenching at the polymer-vacuum interface should be taken into account when the thickness of the polymer film is on the order of the exciton diffusion length; in particular, in the determination of the exciton diffusion length. (*J. Phys. Chem. B* **2009,** *113,* 9104–9109).

Nekoliko primera (ACS author guide)

Nanostructured metallic architectures have unique and highly attractive properties, including large optical field enhancements resulting in strong light scattering and absorption. Modification of prefabricated nanostructures by simple galvanic displacement (GD) allows for the design of new nanomaterials with enhanced optical properties. In this paper, we have studied the optical properties of two families of Ag fractals before and after GD in a Au(III) solution. The new nanomaterials showed significantly improved optical enhancing properties that allowed for straightforward and highly reproducible single-molecule detection by surface-enhanced resonance Raman scattering (SERRS). (*J. Phys. Chem. C* **2009**, *113*, 12897–12900).

Da probamo

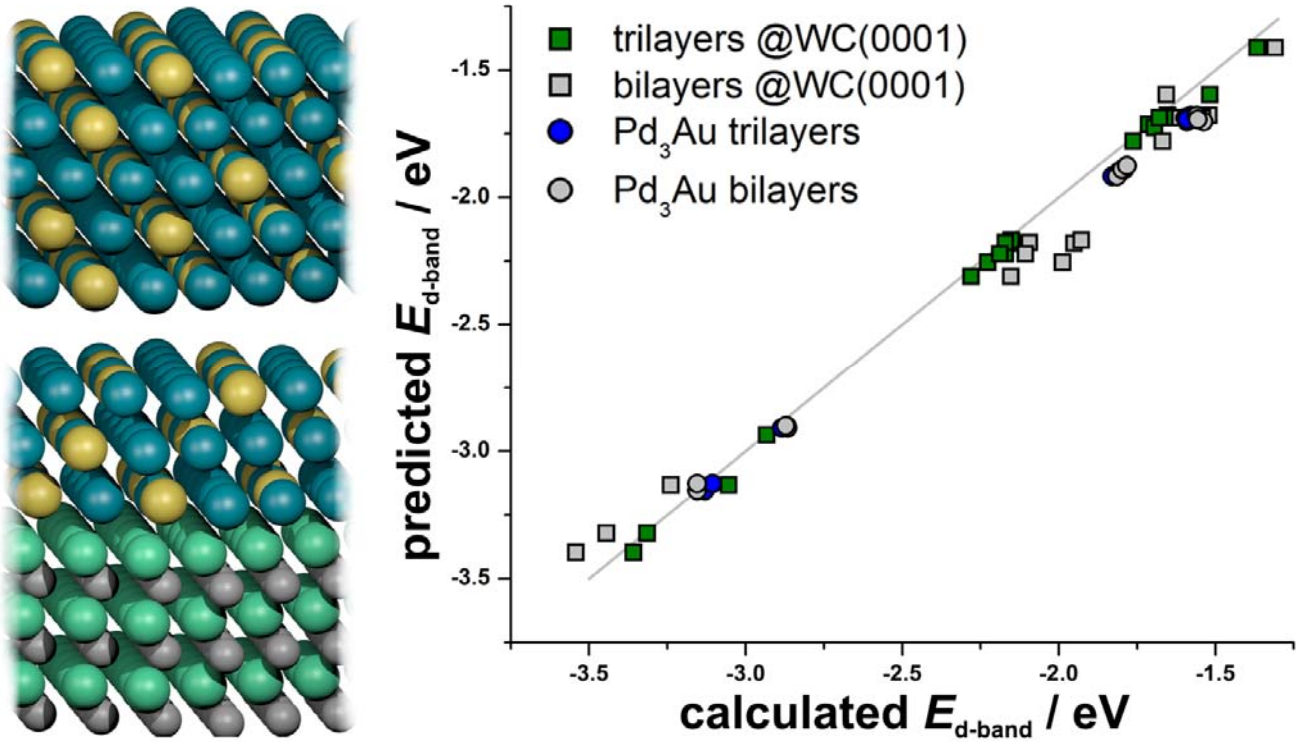
vs.

- **Introduction—what is the topic?**
- **Statement of purpose?**
- **Summarize why have other studies not tackled similar research questions?**
- **How has the research question been tackled?**
- **How was the research done?**
- **What is the key impact of the research?**

Nemojte da...

- Koristite skraćenice
- Izbegavajte reference
- Koristite jednostavan jezik
- Nemojte da kopirate zaključak

OK, sada malo ozbiljnije



Istraživanje

- **Identifikacija tematike/Pretraga literature**
- Postavka eksperimenta
- Izrada eksperimenta
- Analiza i diskusija rezultata
- Priprema publikacije
- Proces publikovanja

Identifikacija teme – predmeta istraživanja

Zašto?

Može li se na osnovu debljine sloja katalizatora na nekoj podlozi predvideti njegovo ponašanje?

Istraživanje

- Identifikacija tematike/Pretraga literature
- **Postavka eksperimenta**
- Izrada eksperimenta
- Analiza i diskusija rezultata
- Priprema publikacije
- Proces publikovanja

Postavka eksperimenta

- Experiment – teško
- *In silico* experiment
- Postavka modela
- Reprezentacija realnog katalizatora
- Reprezentacija modela
- Izbor računske metode

Istraživanje

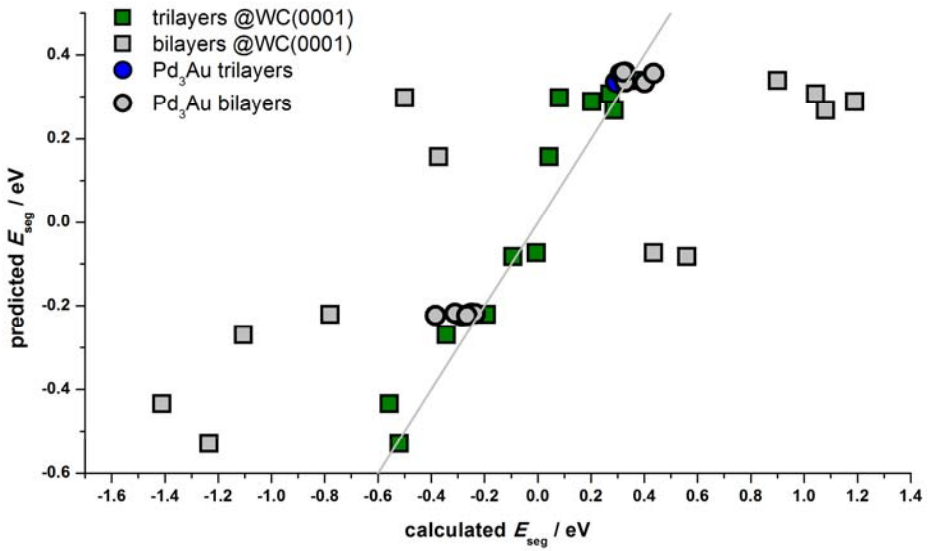
- Identifikacija tematike/Pretraga literature
- Postavka eksperimenta
- **Izrada eksperimenta**
- Analiza i diskusija rezultata
- Priprema publikacije
- Proces publikovanja

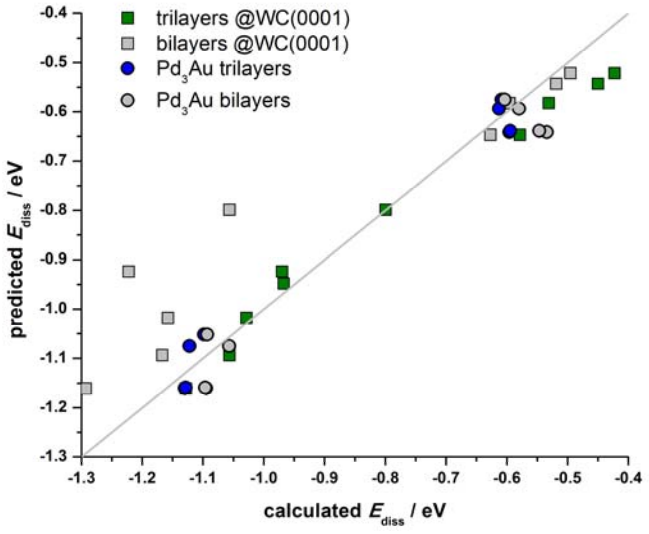
Izrada eksperimenta

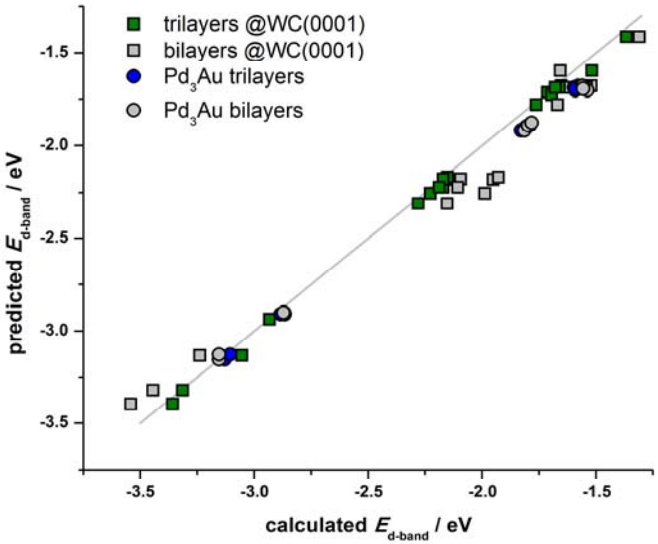
Istraživanje

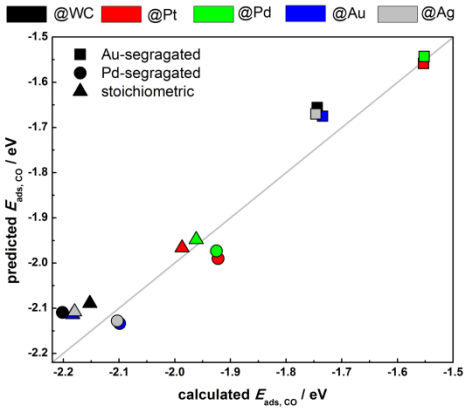
- Identifikacija tematike/Pretraga literature
- Postavka eksperimenta
- Izrada eksperimenta
- **Analiza i diskusija rezultata**
- Priprema publikacije
- Proces publikovanja

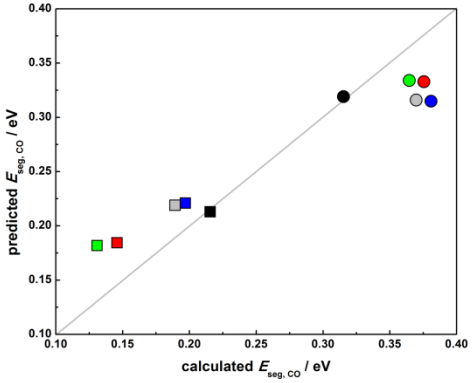
Analiza i diskusija rezultata





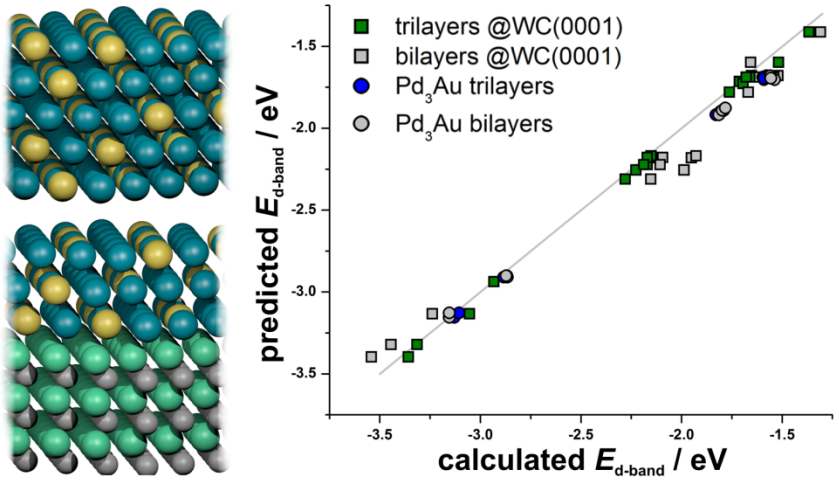






Glavni zaključci su...

Da probamo



- **Introduction—what is the topic?**
- **Statement of purpose?**
- **Summarize why have other studies not tackled similar research questions?**
- **How has the research question been tackled?**
- **How was the research done?**
- **What is the key impact of the research?**

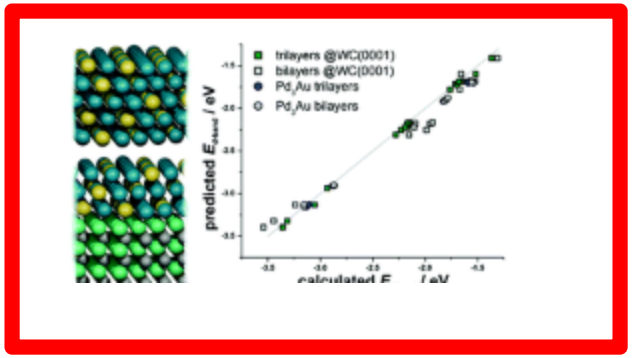
Lattice mismatch as the descriptor of segregation, stability and reactivity of supported thin catalyst films

Edvin Fako[ab] Ana S. Dobrota[a] Igor A. Pašti[*ae] Núria López[b] Slavko V. Mentus[ac] and Natalia V. Skorodumova[de]

Author affiliations

Abstract

The increasing demand and high prices of advanced catalysts motivate a constant search for novel active materials with reduced contents of noble metals. The development of thin films and core–shell catalysts seems to be a promising strategy along this path. Using density functional theory we have analyzed a number of surface properties of supported bimetallic thin films with the composition A_3B (where A = Pt and Pd, and B = Cu, Ag and Au). We focus on the surface segregation, dissolution stability and surface electronic structure. We also address the chemisorption properties of Pd_3Au thin films supported by different substrates, by probing the surface reactivity with CO. We find a strong influence of the support in the case of mono- and bilayers, while the surface strain seems to be the predominant factor in determining the surface properties of supported trilayers and thicker films. In particular, we show that the studied properties of the supported trilayers can be predicted from the lattice mismatch between the overlayer and the support. Namely, if the strain dependence of the corresponding quantities for pure strained surfaces is known, the properties of strained supported trilayers can be reliably estimated. The obtained results can be used in the design of novel catalysts and predictions of the surface properties of supported ultrathin catalyst layers.



ŠTA JE OVO???????

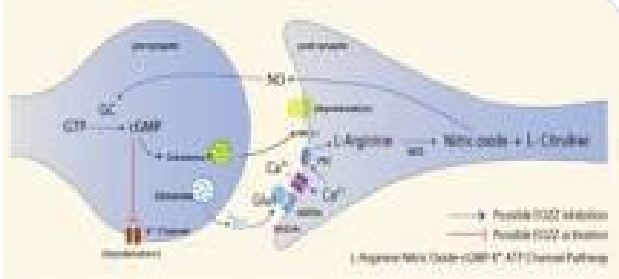
Article type: Paper

DOI: 10.1039/C7CP07276G

Citation: *Phys. Chem. Chem. Phys.*, 2018, 20, 1524-1530

Graphical abstract / Table of Content entry

A **Graphical Abstract** is a single, concise, pictorial and visual summary of the main findings of the article. This could either be the concluding figure from the article or a figure that is specially designed for the purpose, which captures the content of the article for readers at a single glance.



Graphical abstract - Elsevier

https://www.elsevier.com/authors/journal-authors/graphical-abstract

Question Asked 4 years ago

Noble K Kurian
17.26 · Indian Council of Medical Research

How to create a graphical abstract ?

Now most of the journals need graphical abstract for the article to be published. Is there any general guidelines for preparing graphical abstracts ?. Is there any software available design graphical abstracts ?.

All Answers (59)

Linas Balciauskas
Nature Research Centre
4 years ago

First of all - what is the title and text abstract?

3 Recommendations

Linas Balciauskas
Nature Research Centre
4 years ago

Šarolta, it is graphic abstract, not geographic

3 Recommendations

Linas Balciauskas
Nature Research Centre
3 years ago

Idea is most important, not the software

3 Recommendations

Graphical abstract / Table of Content entry

Author instructions

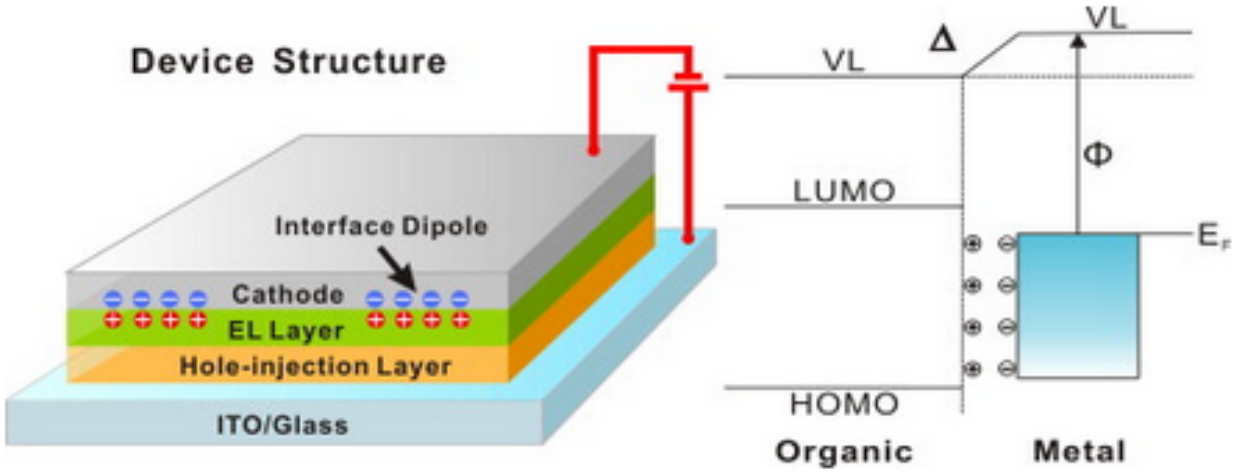
A Graphical Abstract should allow readers to quickly gain an understanding of the main take-home message of the paper and is intended to encourage browsing, promote interdisciplinary scholarship, and help readers identify more quickly which papers are most relevant to their research interests.

Authors must provide an image that clearly represents the work described in the paper. A key figure from the original paper, summarising the content can also be submitted as a graphical abstract.

https://www.elsevier.com/authors/journal-authors/graphical-abstract

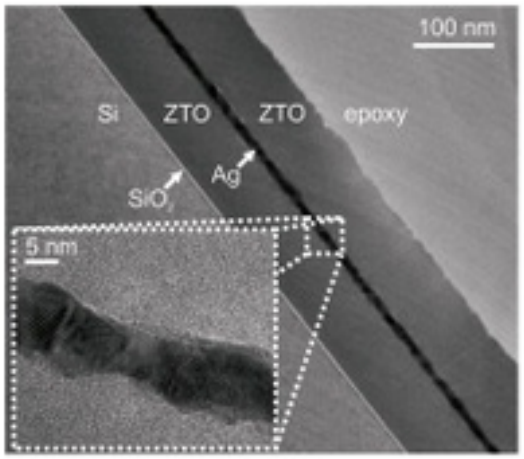
Nekoliko dobrih primera (prema Elsevier-u)

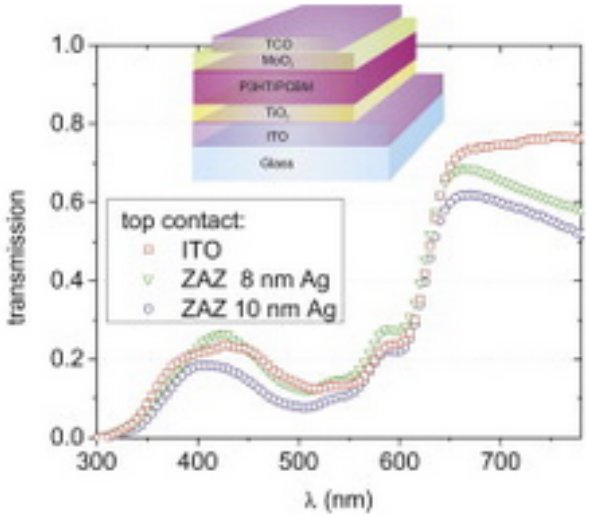
Example 14: Modifying organic/metal interface via solvent treatment to improve electron injection in organic light emitting diodes, Q. Wang, Y. Zhou, Organic Electronics, Volume 12, Issue 11, November 2011, Pages 1858-1863. http://dx.doi.org/10.1016/j.orgel.2011.07.021



Nekoliko dobrih primera (prema Elsevier-u)

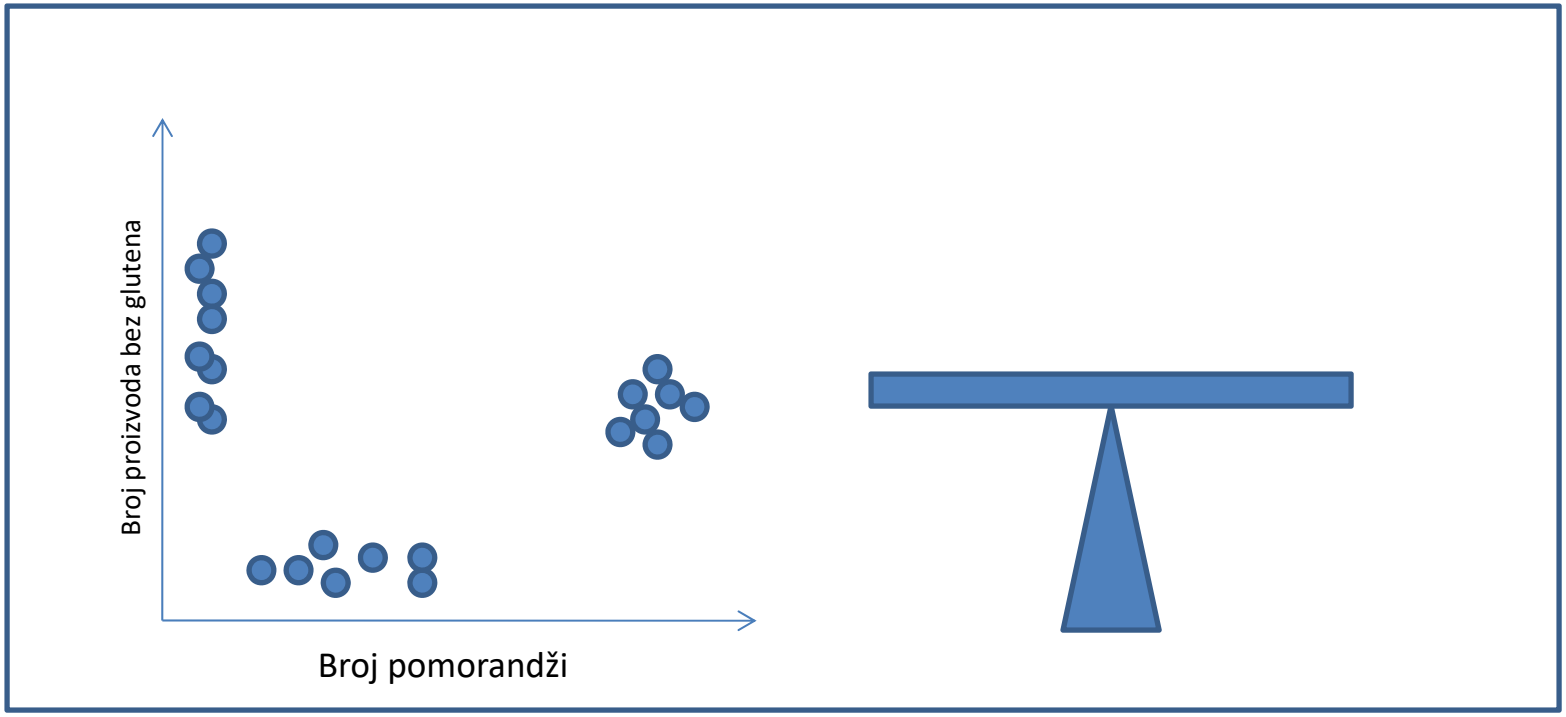
Example 15: Efficient large area semitransparent organic solar cells based on highly transparent and conductive ZTO/Ag/ZTO multilayer top electrodes, Thomas Winkler, Hans Schmidt, et al., Organic Electronics, Volume 12, Issue 10, October 2011, Pages 1612-1618.http://dx.doi.org/10.1016/j.orgel.2011.06.015 ↗





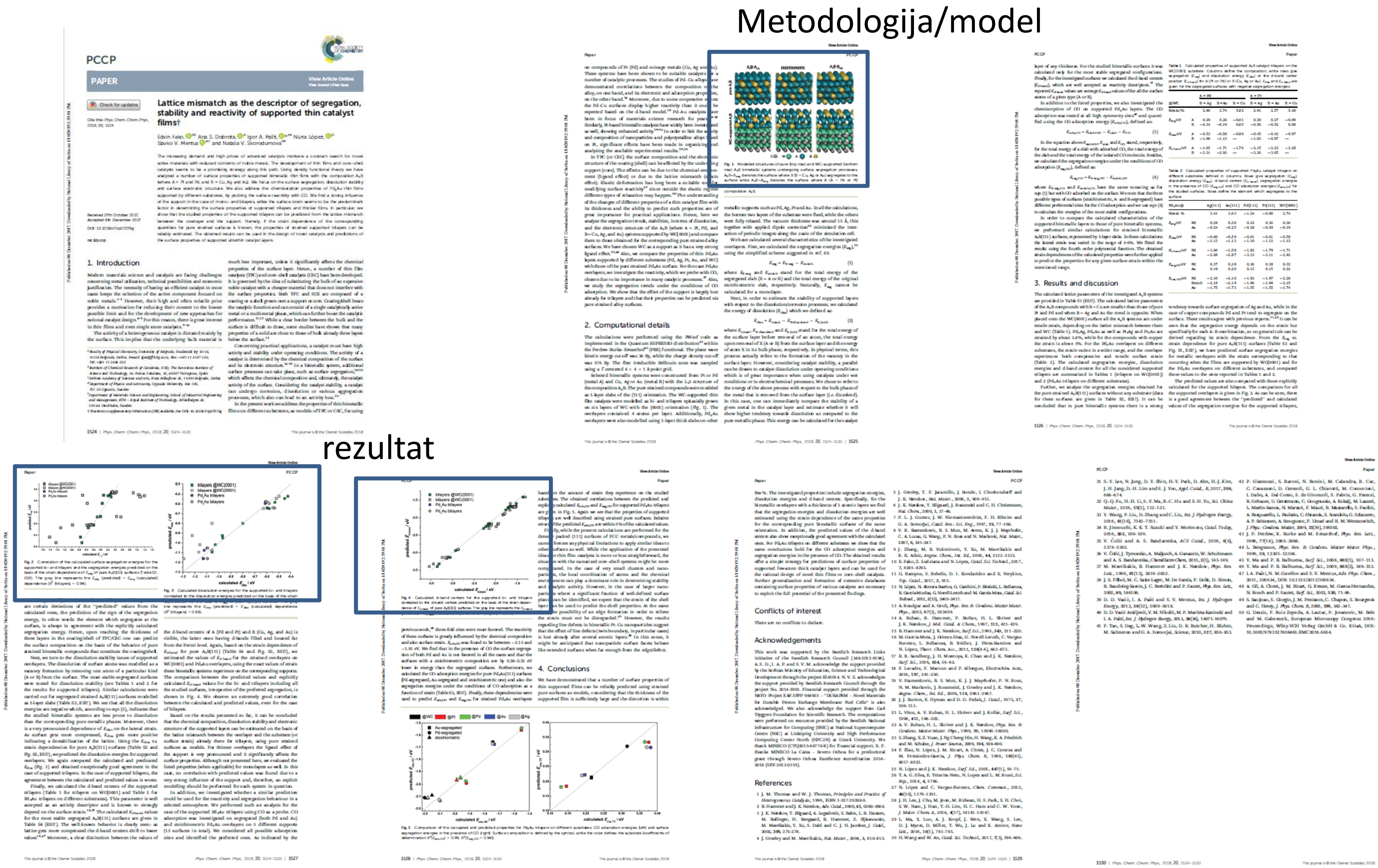
Da probamo

vs.



OK, sada malo ozbiljnije

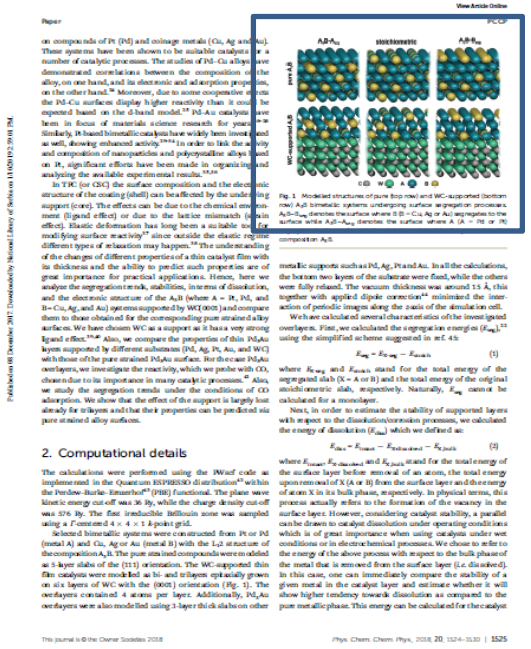
OK, sada malo ozbiljnije

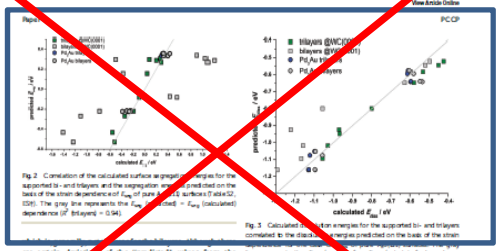


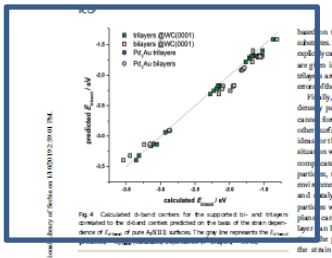
OK, sada malo ozbiljnije

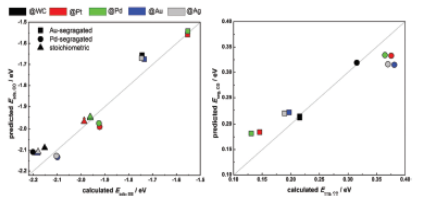
Metodologija/model

rezultat

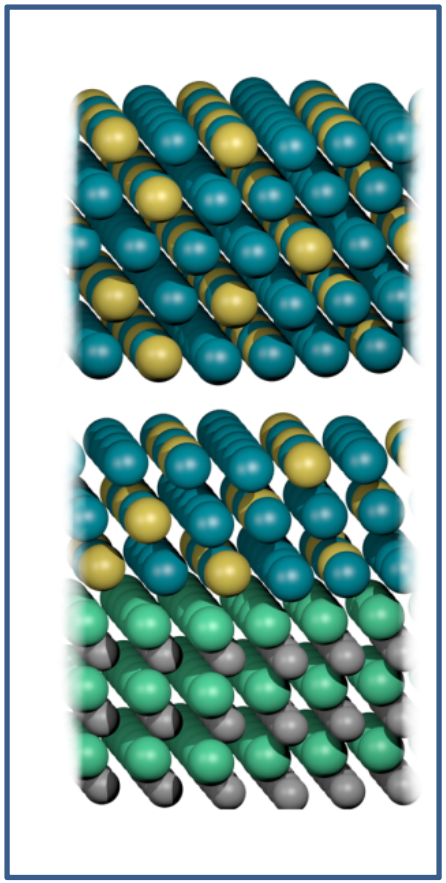




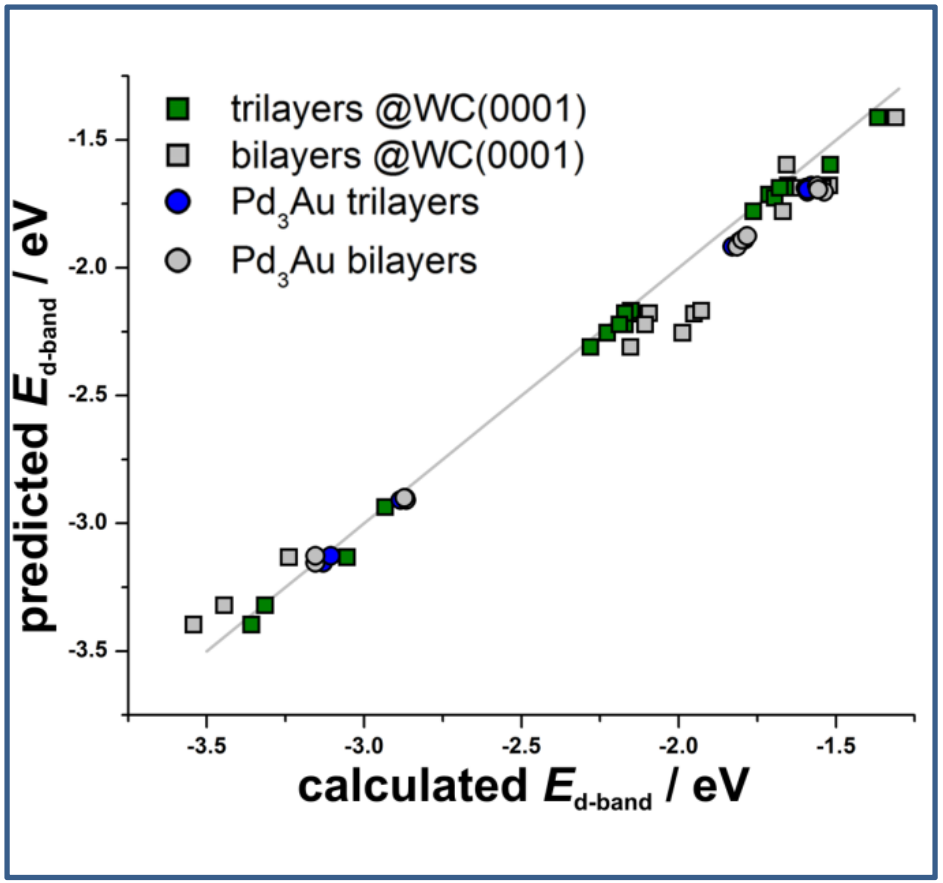




OK, sada malo ozbiljnije



Metodologija/model



rezultat

Istraživanje

- Identifikacija tematike/Pretraga literature
- Postavka eksperimenta
- Izrada eksperimenta
- Analiza i diskusija rezultata
- Priprema publikacije
- **Proces publikovanja**

Proces publikovanja

- Korak 1 – pošaljite manuscript u odabrani časopis

- Po pravilu, časopis će tražiti objašnjenje zašto vaši rezultati treba da budu publikovani baš kod njih.

Cover letter

Question Asked 5 years ago

Subramanyan Namboodiri Varanakkottu
32.34 · National Institute of Technology Calicut

How important is the cover letter when submitting an article to a journal?

Any thoughts/experiences on the importance of cover letters to the editor when submitting a paper? What are the major points we should include there? Do editors reject a paper based on the quality of the covering letter?

Scientific Publication | Journal Articles | Journal Editing | Academic Writing | Peer Review

Linas Balciauskas
Nature Research Centre

5 years ago

Point of view of editor:

-if system asks fpr the cover letter, better to make it not formal, like "please find manuscript fr publication

- if not, I will gladly see cover letter, explaining position of the author about his paper, why journal was chosen, if there is any conflicts of interest, possible reviewers, NOT recommended reviewers and WHY, etc.

- just e-mail and manuscript files make me think, that author do not care about his paper.

6 Recommendations

Cover Letter

Authors must prepare and submit, with their manuscript, a cover letter which includes the following information:

- TITLE OF THE SUBMITTED MANUSCRIPT:
- LIST OF ALL AUTHORS' NAMES AND AFFILIATIONS:
- A SHORT STATEMENT (<50 words) OF THE PRECISE PROBLEM OR OBJECTIVE ADDRESSED IN THE PAPER:
- A VERY BRIEF (<100 words) DESCRIPTION OF THE ESSENCE OF YOUR APPROACH:
- A LIST OF THE SPECIFIC MAJOR NOVEL CONTRIBUTIONS (up to 3) REPORTED HERE:
- LIST OF OTHER JOURNAL OR CONFERENCE PAPERS (if any) PUBISHED OR SUBMITTED BY YOU OR ANY CO-AUTHOR THAT HAVE A SIGNIFICANT OVERLAP WITH THE CONTRIBUTION SUBMITTED HERE ACCOMPANIED BY A BRIEF EXPLANATION OF THE NATURE OF THIS OVERLAP POINTING OUT CLEARLY WHICH NOVEL IDEAS SUBMITTED HERE HAVE NOT BEEN DISCUSSED IN THESE PRIOR PUBLICATIONS:
- A REFERENCE TO THE CLOSEST PRIOR ARTICLE (by others) UPON WHICH YOUR CONTRIBUTIONS IMPROVE:

❖❖❖ Continued ❖❖❖

- THE NAMES, EMAILS, AND HOMEPAGE URLS OF FOUR EXPERTS COVERING THESE AREAS AND FIELDS (by expert, we refer to someone who has published several high quality papers in that technical area in the last five years and who is recognized internationally as an expert in one of the fields you listed above):
- THE NAMES OF THE TWO GMOD ASSOCIATE EDITORS WHO YOU BELIEVE ARE THE MOST QUALIFIED TO HANDLE YOUR PAPER (please go to http://www.elsevier.com/wps/find/journaleditorialboard.cws_home/622839/editorialboard to see list of associate editors:
- TECHNICAL AREAS AND FIELDS OF EXPERTISE NECESSARY TO FULLY UNDERSTAND YOUR CONTRIBUTION AND TO EVALUATE ITS POTENTIAL AND NOVELTY (see list of areas and topics posted at http://ees.elsevier.com/gmod/ and feel free to add areas and fields as needed):

❖❖❖

Cover Letter

Lattice mismatch as the descriptor of segregation, stability and reactivity of supported thin catalyst films

Edvin Fako[ab] Ana S. Dobrota[a] Igor A. Pašti*[ae] Núria López[b] Slavko V. Mentus[ac] and Natalia V. Skorodumova[de]

Author affiliations

Abstract

The increasing demand and high prices of advanced catalysts motivate a constant search for novel active materials with reduced contents of noble metals. The development of thin films and core–shell catalysts seems to be a promising strategy along this path. Using density functional theory we have analyzed a number of surface properties of supported bimetallic thin films with the composition A_3B (where A = Pt and Pd, and B = Cu, Ag and Au). We focus on the surface segregation, dissolution stability and surface electronic structure. We also address the chemisorption properties of Pd_3Au thin films supported by different substrates, by probing the surface reactivity with CO. We find a strong influence of the support in the case of mono- and bilayers, while the surface strain seems to be the predominant factor in determining the surface properties of supported trilayers and thicker films. In particular, we show that the studied properties of the supported trilayers can be predicted from the lattice mismatch between the overlayer and the support. Namely, if the strain dependence of the corresponding quantities for pure strained surfaces is known, the properties of strained supported trilayers can be reliably estimated. The obtained results can be used in the design of novel catalysts and predictions of the surface properties of supported ultrathin catalyst layers.

University of Belgrade
FACULTY OF PHYSICAL CHEMISTRY
www.ffh.bg.ac.rs
Studentski trg 12-16, P.O.Box 47, 11158 Belgrade 118, PAC 105305, Tel: +381 11 2635 345, 3336 625, Fax: +381 11 2187 133, ffh@ffh.bg.ac.rs

University of Belgrade – Faculty of Physical Chemistry
Studentski trg 12-16, 11158 Belgrade, Serbia
e-mail: igor@ffh.bg.ac.rs
Phone: +381 11 3336 625
Fax: +381 11 2187 133

Dear Editor,

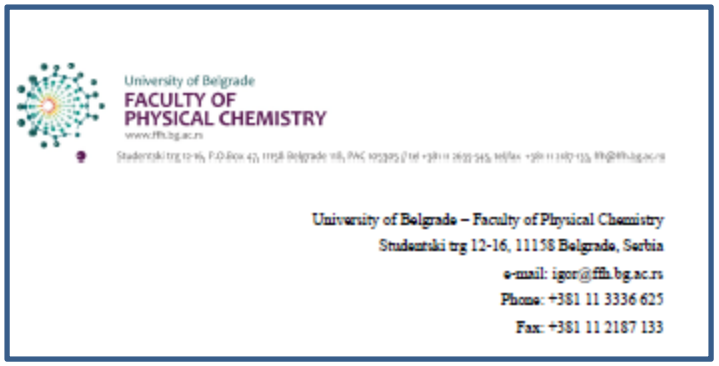
Attached please find the manuscript entitled "Lattice mismatch as the descriptor of segregation, stability and reactivity of supported thin catalyst films" by Fako *et al.* we would like to publish in *Physical Chemistry Chemical Physics*.

Core-shell architectures are crucial to reduce the use of expensive metals in catalysis. Typically the core can be prepared by a cheap material while the shell is the active phase containing one or two metals. By means of Density Functional Theory we have investigated the properties of thin supported bimetallic catalysts films, focusing on the segregation, dissolution and the electronic structure. We show that already for shells formed by alloy trilayers the parameters with decisive role for catalyst performance can be reliably estimated on the basis of lattice mismatch between the support and the overlayer. Namely, by comparing the calculated segregation energies, dissolution energies and the *d*-band centers for the supported bimetallic layers with the estimated ones using the database for pure strained bimetallic systems, we conclude that the effects of support fade for trilayers and supported films behave like pure strained surfaces. We also show that similar conclusion holds for the adsorption as shown when using CO as a probe molecule. We hope that the content of the present manuscript can be of high interest for the readership of *Physical Chemistry Chemical Physics*.

All the authors have agreed on the contents of the manuscript and approved its submission. The article has not been submitted to any other journal. No conflict of interest exists in connection with this article.

With best regards,
Dr. Igor A. Pašti

Cover Letter



University of Belgrade
FACULTY OF
PHYSICAL CHEMISTRY
www.ffh.bg.ac.rs

University of Belgrade – Faculty of Physical Chemistry
Studentski trg 12-16, 11158 Belgrade, Serbia
e-mail: igor@ffh.bg.ac.rs
Phone: +381 11 3336 625
Fax: +381 11 2187 133

Dear Editor,

Attached please find the manuscript entitled "Lattice mismatch as the descriptor of segregation, stability and reactivity of supported thin catalyst films" by Fako *et al.* we would like to publish in *Physical Chemistry Chemical Physics*.

Core-shell architectures are crucial to reduce the use of expensive metals in catalysis. Typically the core can be prepared by a cheap material while the shell is the active phase containing one or two metals. By means of Density Functional Theory we have investigated the properties of thin supported bimetallic catalysts films, focusing on the segregation, dissolution and the electronic structure. We show that already for shells formed by alloy trilayers the parameters with decisive role for catalyst performance can be reliably estimated on the basis of lattice mismatch between the support and the overlayer. Namely, by comparing the calculated segregation energies, dissolution energies and the *d*-band centers for the supported bimetallic layers with the estimated ones using the database for pure strained bimetallic systems, we conclude that the effects of support fade for trilayers and supported films behave like pure strained surfaces. We also show that similar conclusion holds for the adsorption as shown when using CO as a probe molecule. We hope that the content of the present manuscript can be of high interest for the readership of *Physical Chemistry Chemical Physics*.

All the authors have agreed on the contents of the manuscript and approved its submission. The article has not been submitted to any other journal. No conflict of interest exists in connection with this article.

With best regards,
Dr. Igor A. Pašti

Autori imaju instituciju koja stoji iza njih

Cover Letter

University of Belgrade
FACULTY OF
PHYSICAL CHEMISTRY
www.ffh.bg.ac.rs

University of Belgrade – Faculty of Physical Chemistry
Studentski trg 12-16, 11158 Belgrade, Serbia
e-mail: igor@ffh.bg.ac.rs
Phone: +381 11 3336 625
Fax: +381 11 2187 133

Dear Editor,

Attached please find the manuscript entitled "Lattice mismatch as the descriptor of segregation, stability and reactivity of supported thin catalyst films" by Fako *et al.* we would like to publish in *Physical Chemistry Chemical Physics*.

Core-shell architectures are crucial to reduce the use of expensive metals in catalysis. Typically the core can be prepared by a cheap material while the shell is the active phase containing one or two metals. By means of Density Functional Theory we have investigated the properties of thin supported bimetallic catalysts films, focusing on the segregation, dissolution and the electronic structure. We show that already for shells formed by alloy trilayers the parameters with decisive role for catalyst performance can be reliably estimated on the basis of lattice mismatch between the support and the overlayer. Namely, by comparing the calculated segregation energies, dissolution energies and the *d*-band centers for the supported bimetallic layers with the estimated ones using the database for pure strained bimetallic systems, we conclude that the effects of support fade for trilayers and supported films behave like pure strained surfaces. We also show that similar conclusion holds for the adsorption as shown when using CO as a probe molecule. We hope that the content of the present manuscript can be of high interest for the readership of *Physical Chemistry Chemical Physics*.

All the authors have agreed on the contents of the manuscript and approved its submission. The article has not been submitted to any other journal. No conflict of interest exists in connection with this article.

With best regards,
Dr. Igor A. Pašti

Šta bismo hteli

Cover Letter

University of Belgrade
FACULTY OF
PHYSICAL CHEMISTRY
www.ffh.bg.ac.rs

University of Belgrade – Faculty of Physical Chemistry
Studentski trg 12-16, 11158 Belgrade, Serbia
e-mail: igor@ffh.bg.ac.rs
Phone: +381 11 3336 625
Fax: +381 11 2187 133

Dear Editor,

Attached please find the manuscript entitled "Lattice mismatch as the descriptor of segregation, stability and reactivity of supported thin catalyst films" by Fako *et al.* we would like to publish in *Physical Chemistry Chemical Physics*.

Core-shell architectures are crucial to reduce the use of expensive metals in catalysis. Typically the core can be prepared by a cheap material while the shell is the active phase containing one or two metals. By means of Density Functional Theory we have investigated the properties of thin supported bimetallic catalysts films, focusing on the segregation, dissolution and the electronic structure. We show that already for shells formed by alloy trilayers the parameters with decisive role for catalyst performance can be reliably estimated on the basis of lattice mismatch between the support and the overlayer. Namely, by comparing the calculated segregation energies, dissolution energies and the *d*-band centers for the supported bimetallic layers with the estimated ones using the database for pure strained bimetallic systems, we conclude that the effects of support fade for trilayers and supported films behave like pure strained surfaces. We also show that similar conclusion holds for the adsorption as shown when using CO as a probe molecule. We hope that the content of the present manuscript can be of high interest for the readership of *Physical Chemistry Chemical Physics*.

All the authors have agreed on the contents of the manuscript and approved its submission. The article has not been submitted to any other journal. No conflict of interest exists in connection with this article.

With best regards,
Dr. Igor A. Pašti

Zašto i kako

Cover Letter

University of Belgrade
FACULTY OF
PHYSICAL CHEMISTRY
www.ffh.bg.ac.rs

Studentski trg 12-16, P.O.Box 47, 11158 Belgrade 118, PAC 105305 / tel +381 11 2633-336 / fax +381 11 2187-133 / ffh@ffh.bg.ac.rs

University of Belgrade – Faculty of Physical Chemistry
Studentski trg 12-16, 11158 Belgrade, Serbia
e-mail: igor@ffh.bg.ac.rs
Phone: +381 11 3336 625
Fax: +381 11 2187 133

Dear Editor,

Attached please find the manuscript entitled "Lattice mismatch as the descriptor of segregation, stability and reactivity of supported thin catalyst films" by Fako *et al.* we would like to publish in *Physical Chemistry Chemical Physics*.

Core-shell architectures are crucial to reduce the use of expensive metals in catalysis. Typically the core can be prepared by a cheap material while the shell is the active phase containing one or two metals. By means of Density Functional Theory we have investigated the properties of thin supported bimetallic catalysts films, focusing on the segregation, dissolution and the electronic structure. We show that already for shells formed by alloy trilayers the parameters with decisive role for catalyst performance can be reliably estimated on the basis of lattice mismatch between the support and the overlayer. Namely, by comparing the calculated segregation energies, dissolution energies and the *d*-band centers for the supported bimetallic layers with the estimated ones using the database for pure strained bimetallic systems, we conclude that the effects of support fade for trilayers and supported films behave like pure strained surfaces. We also show that similar conclusion holds for the adsorption as shown when using CO as a probe molecule. We hope that the content of the present manuscript can be of high interest for the readership of *Physical Chemistry Chemical Physics*.

All the authors have agreed on the contents of the manuscript and approved its submission. The article has not been submitted to any other journal. No conflict of interest exists in connection with this article.

With best regards,
Dr. Igor A. Pašti

Rezultati

Cover Letter

University of Belgrade – Faculty of Physical Chemistry
Studentski trg 12-16, 11158 Belgrade, Serbia
e-mail: igor@ffh.bg.ac.rs
Phone: +381 11 3336 625
Fax: +381 11 2187 133

Dear Editor,

Attached please find the manuscript entitled "Lattice mismatch as the descriptor of segregation, stability and reactivity of supported thin catalyst films" by Fako *et al.* we would like to publish in *Physical Chemistry Chemical Physics*.

Core-shell architectures are crucial to reduce the use of expensive metals in catalysis. Typically the core can be prepared by a cheap material while the shell is the active phase containing one or two metals. By means of Density Functional Theory we have investigated the properties of thin supported bimetallic catalysts films, focusing on the segregation, dissolution and the electronic structure. We show that already for shells formed by alloy trilayers the parameters with decisive role for catalyst performance can be reliably estimated on the basis of lattice mismatch between the support and the overlayer. Namely, by comparing the calculated segregation energies, dissolution energies and the *d*-band centers for the supported bimetallic layers with the estimated ones using the database for pure strained bimetallic systems, we conclude that the effects of support fade for trilayers and supported films behave like pure strained surfaces. We also show that similar conclusion holds for the adsorption as shown when using CO as a probe molecule. We hope that the content of the present manuscript can be of high interest for the readership of *Physical Chemistry Chemical Physics*.

All the authors have agreed on the contents of the manuscript and approved its submission. The article has not been submitted to any other journal. No conflict of interest exists in connection with this article.

With best regards,
Dr. Igor A. Pašti

Malo pohvalite časopis

Cover Letter

University of Belgrade
FACULTY OF
PHYSICAL CHEMISTRY
www.ffh.bg.ac.rs

University of Belgrade – Faculty of Physical Chemistry
Studentski trg 12-16, 11158 Belgrade, Serbia
e-mail: igor@ffh.bg.ac.rs
Phone: +381 11 3336 625
Fax: +381 11 2187 133

Dear Editor,

Attached please find the manuscript entitled "Lattice mismatch as the descriptor of segregation, stability and reactivity of supported thin catalyst films" by Fako *et al.* we would like to publish in *Physical Chemistry Chemical Physics*.

Core-shell architectures are crucial to reduce the use of expensive metals in catalysis. Typically the core can be prepared by a cheap material while the shell is the active phase containing one or two metals. By means of Density Functional Theory we have investigated the properties of thin supported bimetallic catalysts films, focusing on the segregation, dissolution and the electronic structure. We show that already for shells formed by alloy trilayers the parameters with decisive role for catalyst performance can be reliably estimated on the basis of lattice mismatch between the support and the overlayer. Namely, by comparing the calculated segregation energies, dissolution energies and the *d*-band centers for the supported bimetallic layers with the estimated ones using the database for pure strained bimetallic systems, we conclude that the effects of support fade for trilayers and supported films behave like pure strained surfaces. We also show that similar conclusion holds for the adsorption as shown when using CO as a probe molecule. We hope that the content of the present manuscript can be of high interest for the readership of *Physical Chemistry Chemical Physics*.

All the authors have agreed on the contents of the manuscript and approved its submission. The article has not been submitted to any other journal. No conflict of interest exists in connection with this article.

With best regards,
Dr. Igor A. Pašti

Tehnički detalji, etika u publikovanju

Da probamo

vs.

The University of Maximegalon
Maximegalon Institute of Slowly and Painfully Working Out the Surprisingly Obvious

Poštovani/Dragi Uredniče,

…

Zaključak

- Prodajte svoju priču najbolje što znate
- Nauka je

Krv, Sreća,
Suze i Znoj