

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

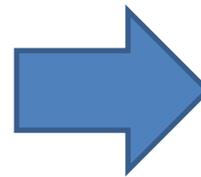
Postavka eksperimenta

- 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

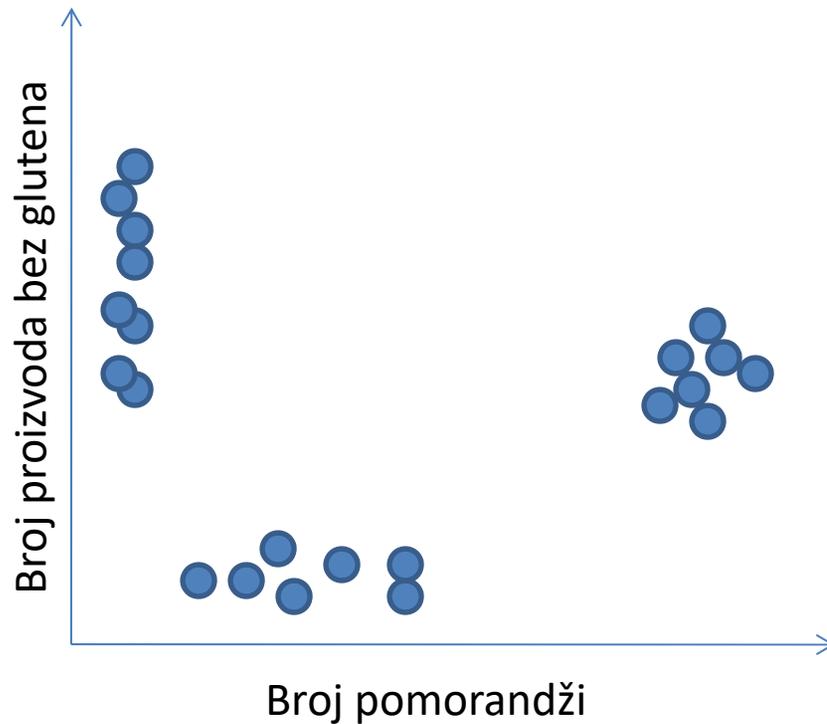
Izrada eksperimenta



Istraživanje

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

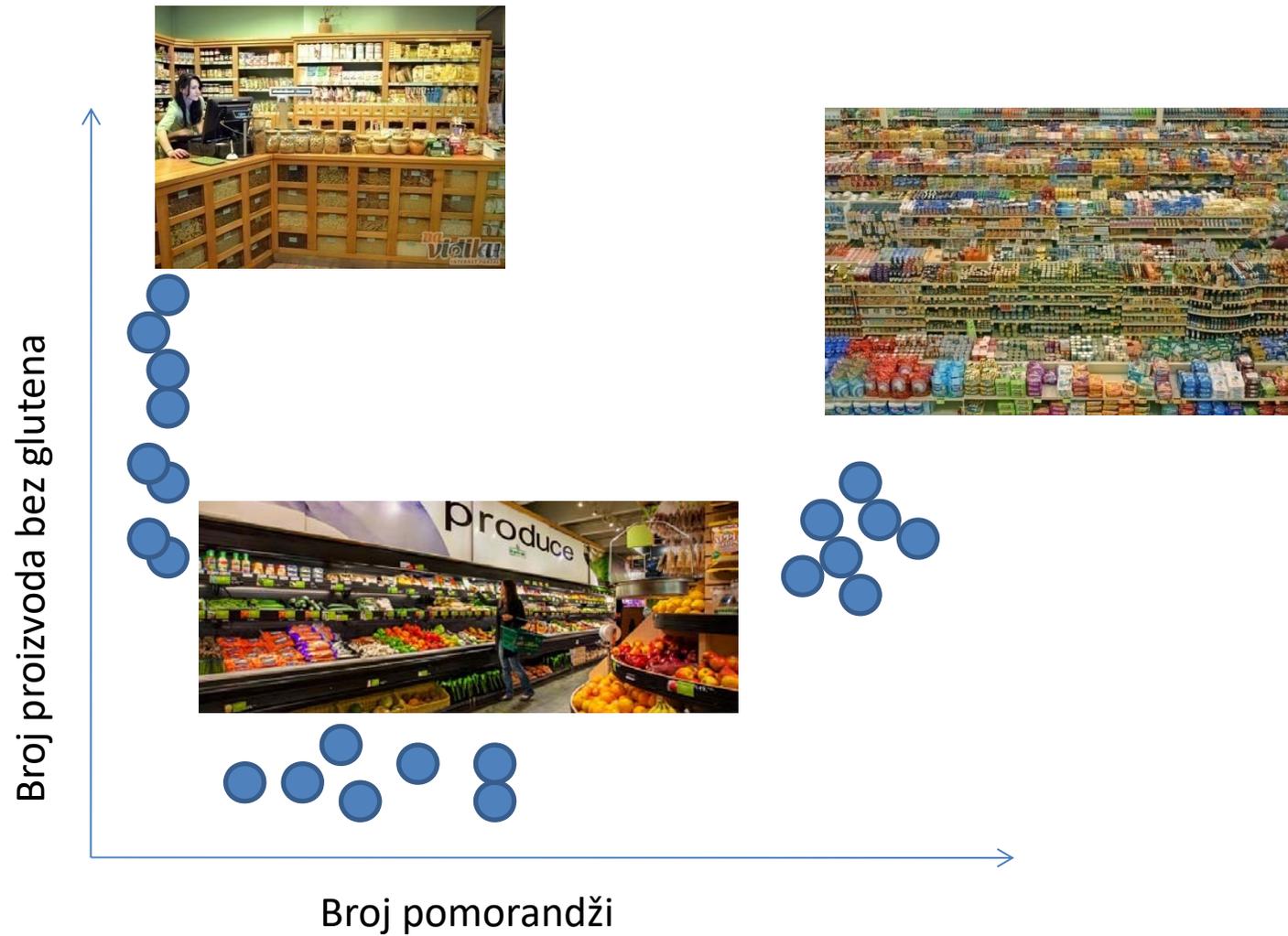
Analiza i diskusija rezultata



Zaključci:

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

Analiza i diskusija rezultata



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

WRITING SCIENTIFIC PAPERS/research articles



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](https://doi.org/10.4103/0019-5545.82558)

PMCID: PMC3136027

PMID: [21772657](https://pubmed.ncbi.nlm.nih.gov/21772657/)

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

[Chittaranjan Andrade](#)

▸ [Author information](#) ▸ [Copyright and License information](#) [Disclaimer](#)

This article has been [cited by](#) other articles in PMC.

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.”

Tipovi abstrakta

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

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)

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

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).

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

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*

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?

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



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
- Reprerzentacija realnog katalizatora
- Reprerzentacija modela
- Izbor računrske metode

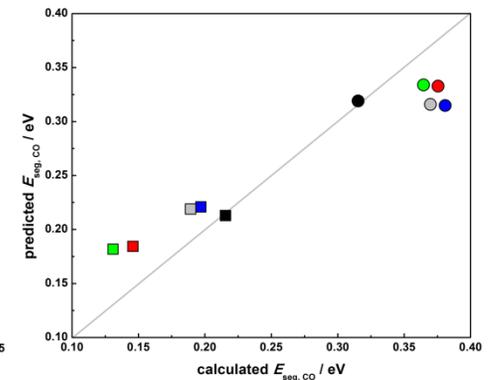
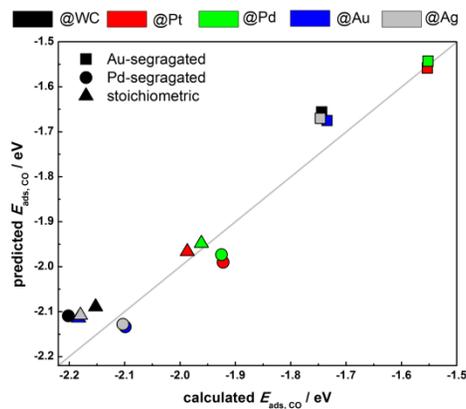
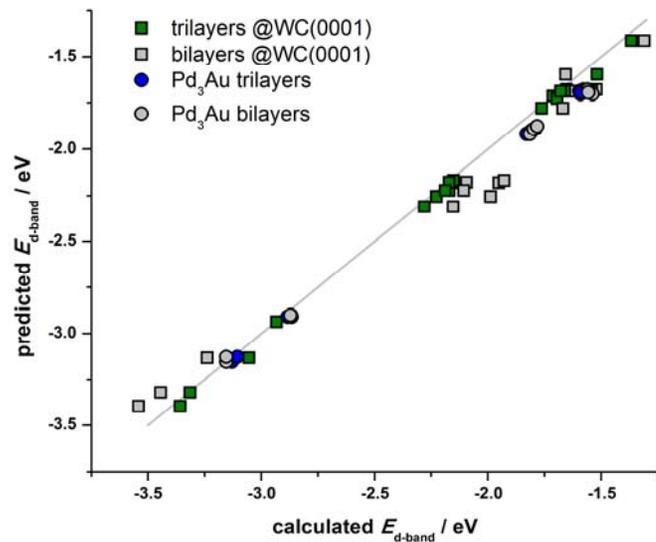
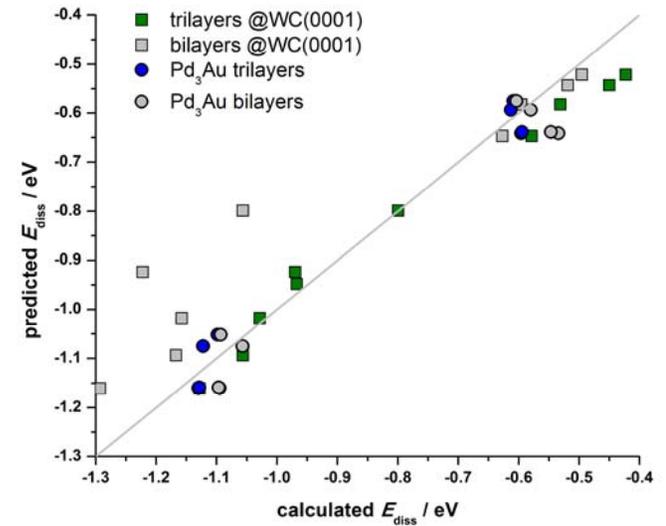
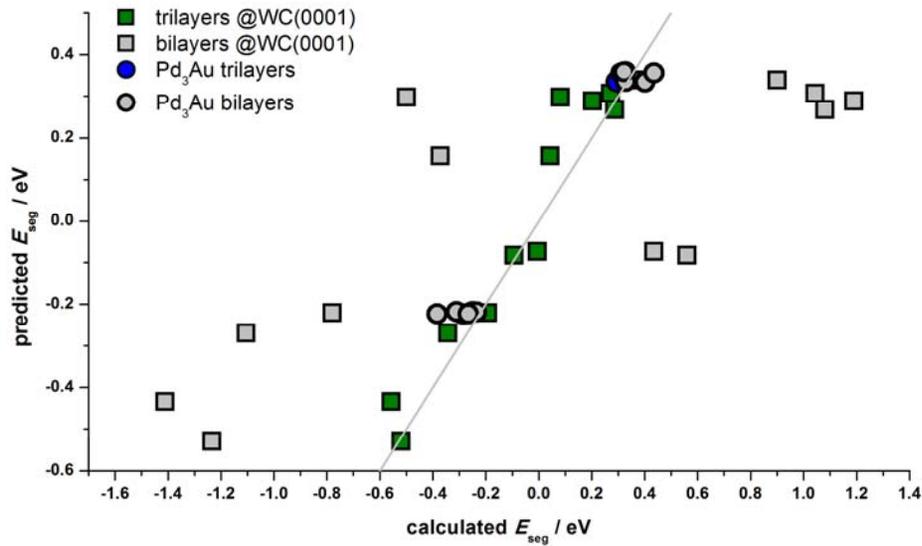
Istraživanje

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

Istraživanje

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

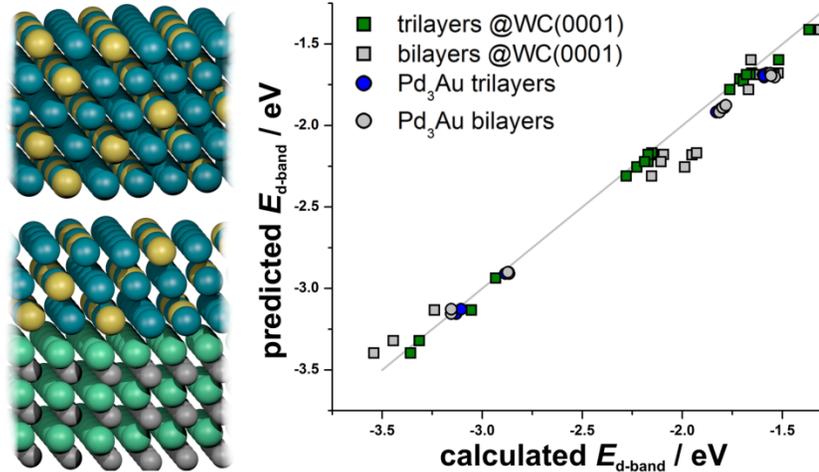
Analiza i diskusija rezultata



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

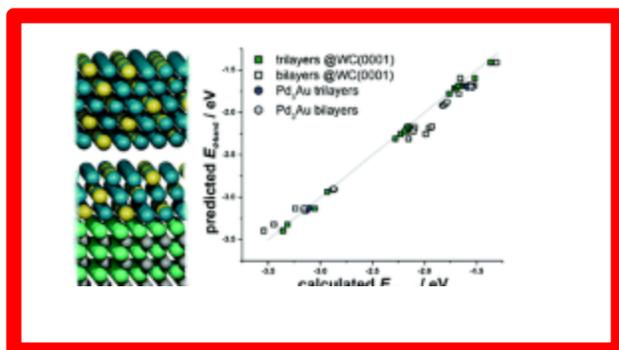


Edvin Fako^{ab}, Ana S. Dobrota^a, Igor A. Pašti^{*ac}, Núria López^b, Slavko V. Mentus^{ac} and Natalia V. Skorodumova^{de}

⊕ 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 $A = \text{Pt}$ and Pd , and $B = \text{Cu}$, 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 HTML

Supplementary files

Supplementary information
PDF (489K)

Publication details



The article was received on 27 Oct 2017, accepted on 08 Dec 2017 and first published on 08 Dec 2017

Tweet

Share

Article type: Paper

DOI: 10.1039/C7CP07276G

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

BibTex

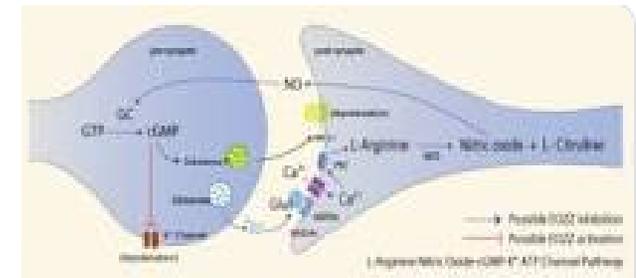
Go

Request permissions

Search articles by author

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

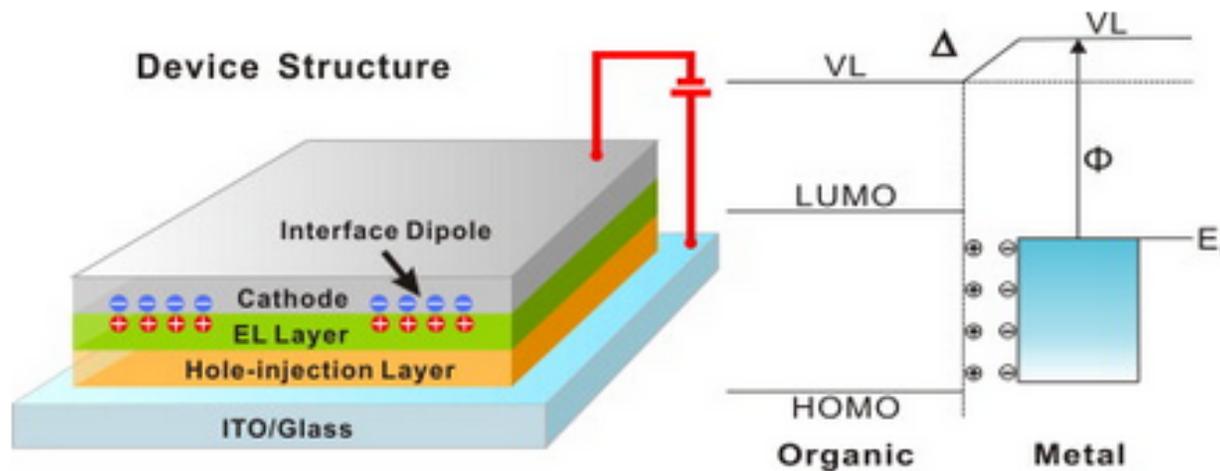
Author instructions

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.

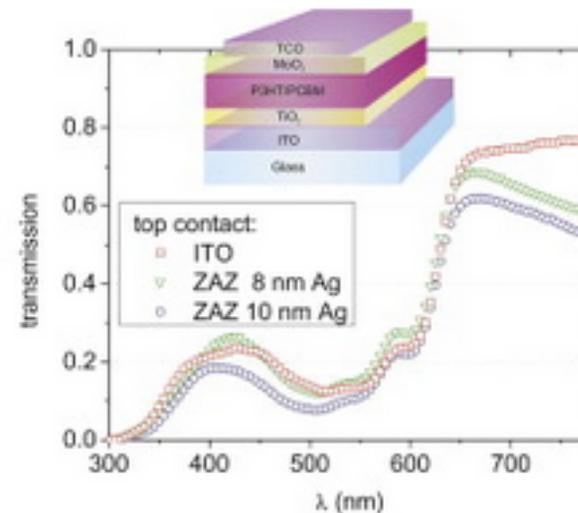
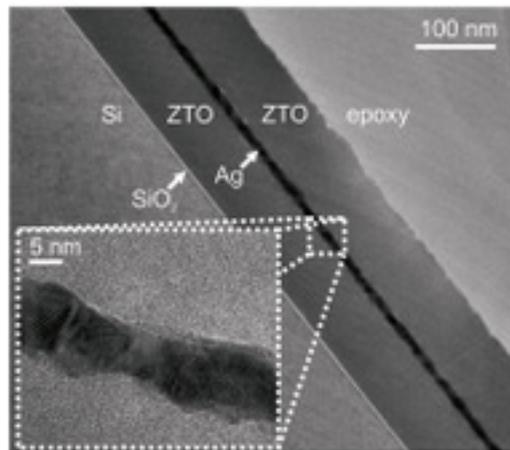
Nekoliko dobrih primera (prema Elsevier-u)

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)

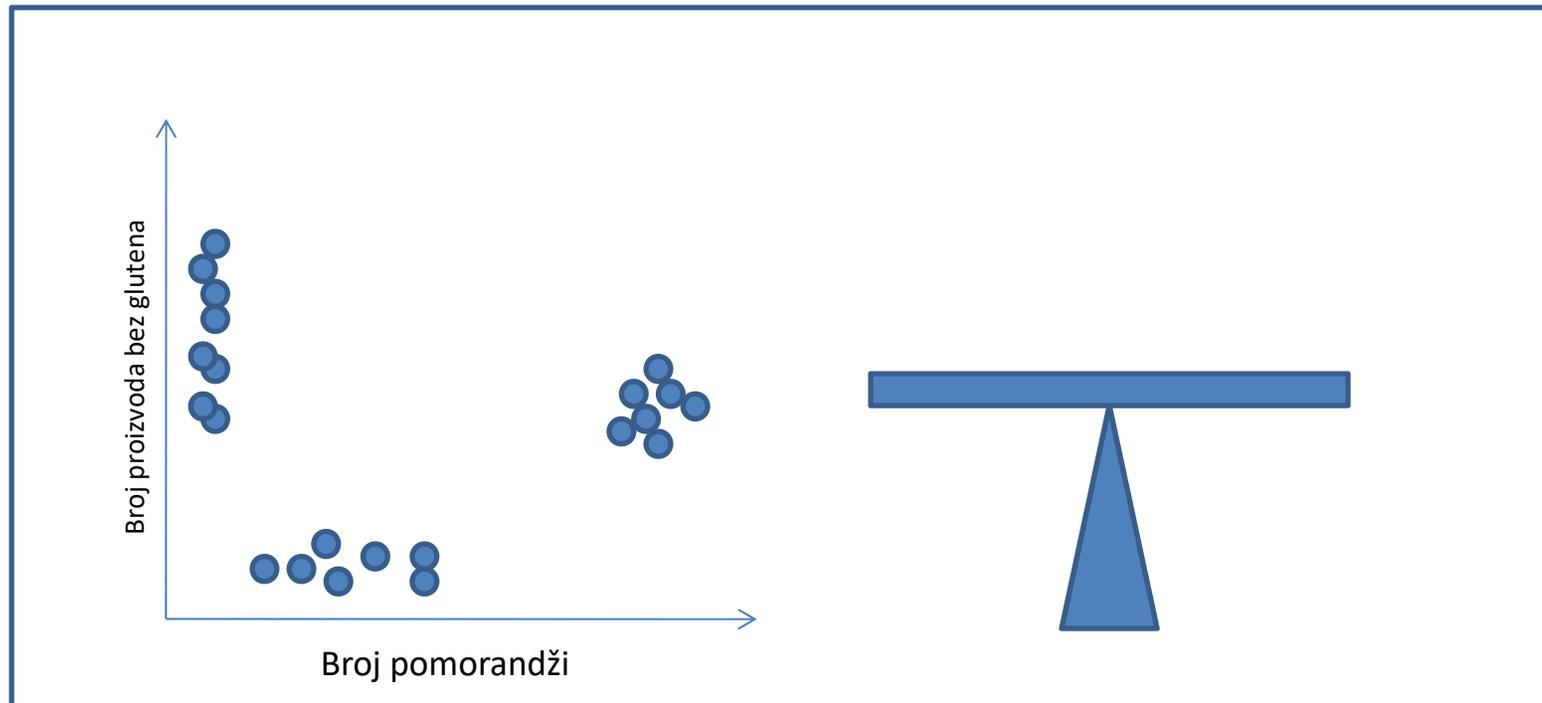
Example 15: Efficient large area semitransparent organic solar cells based on highly transparent and conductive ZTO/Ag/ZTO multilayer top electrodes, Thomas Winkler, Hans Schmidt, et al., Organic Electronics, Volume 12, Issue 10, October 2011, Pages 1612-1618.<http://dx.doi.org/10.1016/j.orgel.2011.06.015>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



Da probamo



vs.



OK, sada malo ozbiljnije

Metodologija/model

rezultat

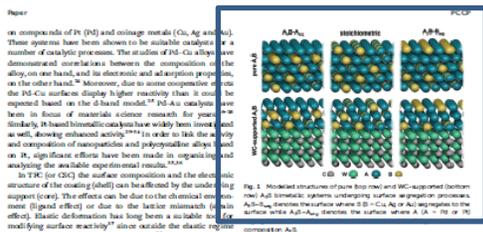


Fig. 1. Molecular structures of pure Pt and WC-supported bimetallic Pt-Au bimetallic systems.

on compounds of Pt (Pd) and coinage metals (Cu, Ag, Au). These systems have been shown to be suitable catalysts for a number of catalytic processes. The studies of Pt-Cu alloys have demonstrated correlations between the composition of the alloy, on one hand, and its electronic and adsorption properties, on the other hand.¹⁸ Moreover, due to some cooperation on the Pt-Cu surface, display higher reactivity than it could be expected based on the d-band model.¹⁹ Pd-Au catalysts have been in focus of materials science research for years.²⁰ Similarly, Pt-based bimetallic systems have widely been investigated as well, drawing enhanced activity^{21,22} in order to link the activity and composition of nanoparticles and polynanoparticle alloys.²³ In Pt, significant efforts have been made in organic and analyzing the available experimental results.^{24,25} In Pt-C (Pt-Cu) the surface composition and the electronic structure of the coating (shell) can be affected by the underlayer support (overlayer). The effects can be due to the chemical environment (ligand effect) or due to the lattice mismatch (strain effect). Elastic deformation has long been a suitable way to modify surface reactivity²⁶ since outside the elastic regime different types of relaxation may happen.²⁷ The understanding of the charges of different properties of thin catalytic films with its thickness and the ability to predict such properties are of great importance for practical applications. Hence, here we analyze the segregation, strain, stability, trends of dissociation, and the electronic structure of the A_nB_m (where $A = Pt, Pd$, and $B = Cu, Ag$, and Au) systems supported by WC(0001) and compare them to those obtained for the corresponding pure strained alloy surfaces. We have chosen WC as a support as it has a very strong ligand effect.²⁸ Also, we compare the properties of thin PtAu layers supported by different substrates (Pt, Ag, Pt, Au, and WC) with those of the pure strained PtAu surface. For the case of PtAu overlayers, we investigate the reactivity, which we probe with CO, due to its role as a probe in many catalytic processes.²⁹ Also, we study the segregation trends under the conditions of CO adsorption. We show that the effect of the support is largely less already for trilayers and that a proportion can be predicted for pure strained alloy surfaces.

2. Computational details

The calculations were performed using the VASP code as implemented in the Quantum ESPRESSO distribution³⁰ within the Prowler-Block-Elasticity³¹ (PBE) functional. The plane wave kinetic energy cut-off was 36 Ry, while the charge density cut-off was 376 Ry. The first irreducible Brillouin zone was sampled using a Γ -centered $4 \times 4 \times 1$ point grid. Selected bimetallic systems were constructed from Pt or Pd (metal A) and Cu, Ag or Au (metal B) with the $1 \times 1 \times 1$ structure of the decomposition A_nB_m . The point sites used corresponded were defined as n layer slabs of the (111) orientation. The WC-supported thin film catalysts were modeled as bi- and trilayers periodically grown on six layers of WC with the (0001) orientation (Fig. 1). The overlayers contained 4 atoms per layer. Additionally, PtAu overlayers were also modeled using 3-layer thin slabs on other

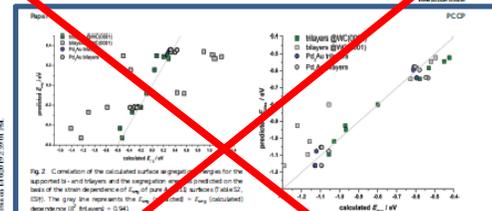


Fig. 2. Correlation of the calculated surface segregation energy for the supported bi- and trilayers and the segregation energy predicted on the basis of the strain dependence of E_{sep} of pure metal surfaces (Table 2, ESI). The grey line represents the $E_{sep}^0 = E_{sep}^0$ (isolated) dependence (E_Sep = 0.5E_Sep).

are certain deviations of the "predicted" values from the calculated ones. In search of the origin of the segregation energy, we always in agreement with the explicitly calculated segregation energy. Hence, upon reaching the thickness of 3 layers in the case of PtAu(111) on WC(0001) one can predict the surface composition on the basis of the behavior of pure strained bimetallic compounds that constitute the catalysts. Next, we turn to the dissociation stability issues of supported overlayers. The dissociation of surface atoms was modeled as a vacancy formation by removing one atom of a particular kind (A or B) from the surface. The most stable segregated surface was used for dissociation stability (see Tables 1 and 2 for the results for supported trilayers). Similar calculations were carried out for segregated strained Au(111) surfaces modeled as 1-layer slabs (Table S1, ESI). We note that all the dissociation energies are negative which, according to (2), indicates that the studied bimetallic systems are less prone to dissociation than the corresponding pure metallic phases. Moreover, there is a very pronounced dependence of E_{diss} on the lateral strain. As surface gets more compressed, E_{diss} gets more positive indicating a destabilization of the lattice. Using the E_{diss} vs strain dependencies for pure Au(111) surfaces (Table S1 and Fig. S2, ESI), we predicted the dissociation energy for supported overlayers. We again compared the calculated and predicted E_{diss} (Fig. 3) and obtained exceptionally good agreement in the case of supported trilayers. In the case of supported bilayers, the agreement between the calculated and predicted values is worse.

Finally, we calculated the d-band centers of the supported overlayers (Table 1 for trilayers on WC(0001) and Table 2 for PtAu overlayers on different substrates). This parameter is well accepted as an activity descriptor and is known to strongly depend on the surface strain.³² The calculated E_{d-band} values for the most stable segregated Au(111) surfaces are given in Table S4 (ESI). The well-known behavior is clearly seen as being the more compressed the d-band centers shift to lower values.³³ Moreover, a clear distinction between the values of

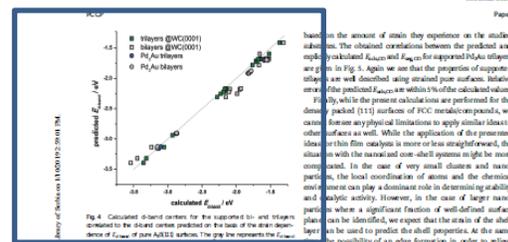


Fig. 3. Calculated d-band centers for the supported bi- and trilayers compared to the d-band centers predicted on the basis of the strain dependence of E_{sep} of pure metal surfaces (Table 2, ESI). The grey line represents the $E_{d-band}^0 = E_{d-band}^0$ (isolated) dependence (E_d-band = 0.5E_d-band).

of the amount of strain they experience on the studied surfaces. The obtained correlations between the predicted and explicitly calculated E_{d-band} and E_{sep} for supported PtAu overlayers are given in Fig. 5. Again we see that the properties of supported overlayers are well described using strained pure surface. Bimetallic (Pt-Au) overlayers are within 5% of the calculated values. Finally, while the present calculations are performed for the densely packed (111) surfaces of PtAu overlayers, we can also consider any physical limitations to apply similar ideas to other surfaces as well. While the application of the present ideas in thin film catalysis is more or less straightforward, the situation with the nanoscale core-shell systems might be more complicated. In the case of very small clusters and nanoparticles, the local coordination of atoms and the chemical environment can play a dominant role in determining stability and catalytic activity. However, in the case of larger nanoparticles where a significant fraction of well-defined surface planes can be identified, we expect that the strain of the shell layer can be used to predict the shell properties. At the same time, the possibility of an edge formation in order to relieve the strain must not be disregarded.³⁴ However, the results regarding line defects in bimetallic Pt-Cu nanoparticles suggest that the effect of line defects (with boundary, in particular case) is less already after several atomic layers.³⁵ In this sense, it might be anticipated that nanoparticle surface facets behave like extended surfaces when far enough from the algorithm.

4. Conclusions

We have demonstrated that a number of surface properties of supported films can be reliably predicted using strained pure surfaces as models, considering that the thickness of the supported film is sufficiently large and the distortion is within

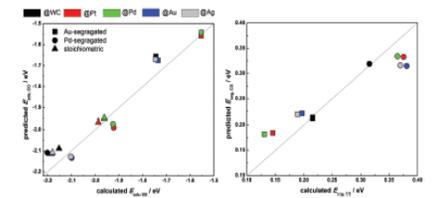
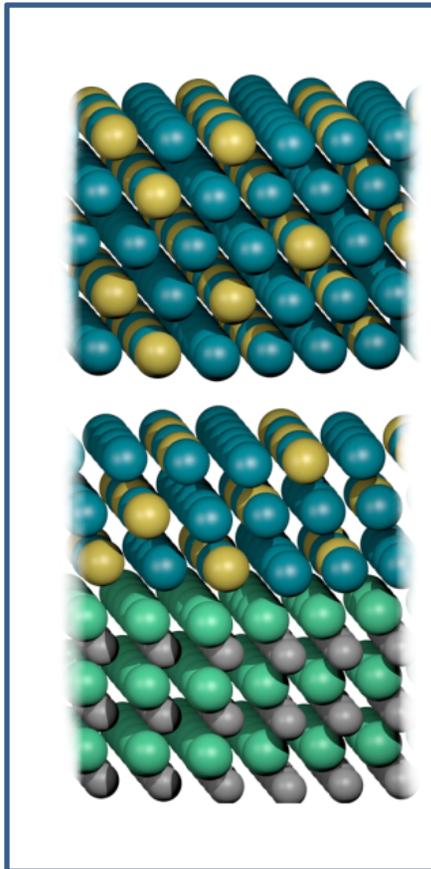
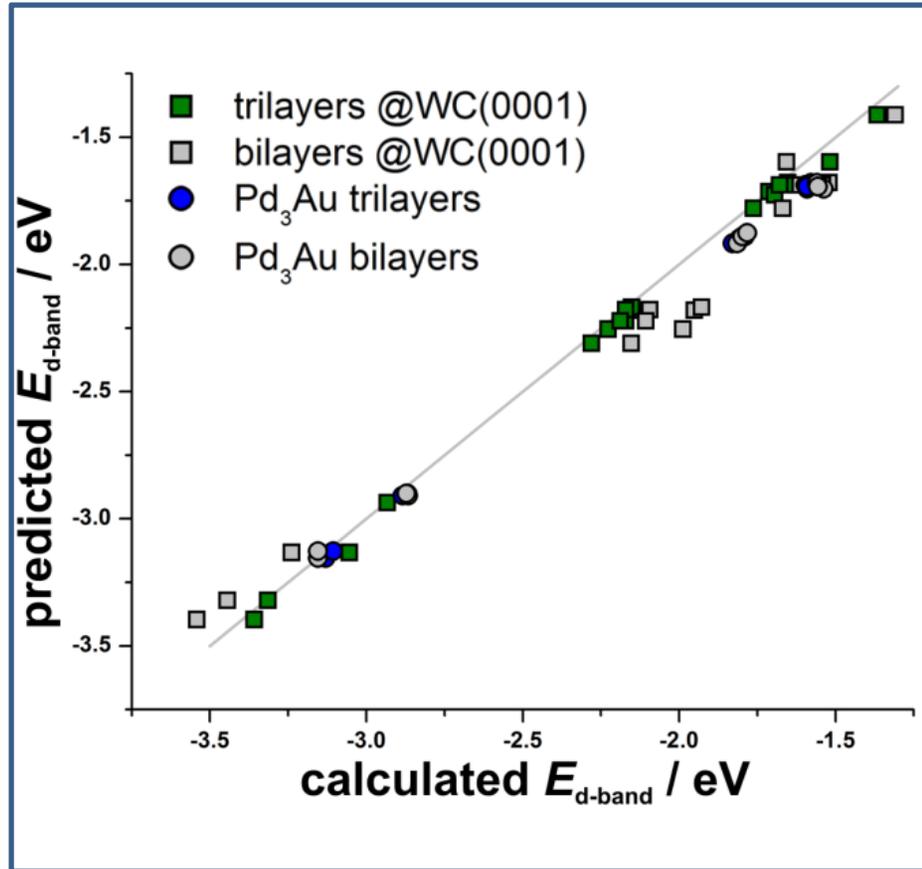


Fig. 4. Comparison of the calculated and predicted properties for PtAu overlayers on different substrates. CO adsorption energy (E_{ad}) and surface segregation energies in the presence of CO (PtAu). Surface composition is defined by the symbols while the color refers to the substrate coefficients of determination ($R^2 = 0.99$, $R^2_{CO} = 0.94$).

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 for the cover letter, better to make it not formal, like "please find manuscript for 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) PUBLISHED 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^{a,b}, Ana S. Dobrota^a, Igor A. Pašti^{*a,c}, 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 $A = \text{Pt}$ and Pd , and $B = \text{Cu}$, 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.fh.bg.ac.rs

Studentski trg 12-16, P.O. Box 47, 1108 Belgrade 16, PK 10229/21 of +381 11 3336 625, 11081 +381 11 2187 133, fh@fh.bg.ac.rs

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

Dear Editor,

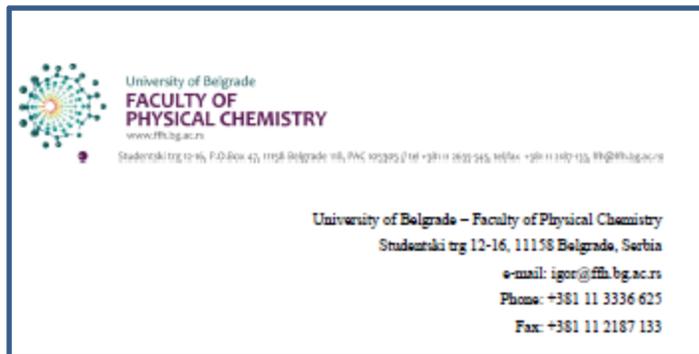
Attached please find the manuscript entitled “Lattice mismatch as the descriptor of segregation, stability and reactivity of supported thin catalyst films” by Fako *et al.* we would like to publish in *Physical Chemistry Chemical Physics*.

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



Autori imaju instituciju koja stoji iza njih

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. Patti

Cover Letter



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

Studentski trg 12-16, P.O. Box 47, 11158 Belgrade 48, PAC 303307 (tel: +381 11 333 625, 6254; fax: +381 11 337 133, 133) fh@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. Patti

Šta bismo hteli

Cover Letter



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

Studentski trg 12-16, P.O. Box 47, 11158 Belgrade 98, PAC 323292106 +381 11 3336 625, 10/16 +381 11 337 133, fh@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. Patti

Zašto i kako

Cover Letter



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

Studentski trg 12-16, P.O. Box 47, 11158 Belgrade 48, PAC 103357 / tel: +381 11 333 625, 103358 / fax: +381 11 337 133, fh@fhbg.ac.rs

University of Belgrade – Faculty of Physical Chemistry
Studentski trg 12-16, 11158 Belgrade, Serbia
e-mail: igor@fh.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 overlay. 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. Patti

Rezultati

Cover Letter



University of Belgrade – Faculty of Physical Chemistry
Studentski trg 12-16, 11158 Belgrade, Serbia
e-mail: igor@fh.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. Patti

Malo pohvalite časopis

Cover Letter



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

Studentski trg 12-16, P.O. Box 47, 11158 Belgrade 98, P.M. 102292 (tel: +381 11 333 625, 625; fax: +381 11 337 133, 133) fh@fhbg.ac.rs

University of Belgrade – Faculty of Physical Chemistry
Studentski trg 12-16, 11158 Belgrade, Serbia
e-mail: igor@fh.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. Patti

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**

