# Spectroscopic study of ultrathin layers formed on metal single crystal surfaces

*PhD. Theses*

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# 1. <u>Introduction</u>

In the twenty-first century, humanity has to face a myriad of challenges, some of which were already known to the well-intelligenced segments of society, but with the widespread use of Internet, these problems became obvious to all. The biggest tasks include the exploration and development of renewable energy sources, reduction of $CO_2$ emission and atmospheric concentration, elaboration of more efficient and environmentally more friendly energy storage concepts, development of new types of material systemsand further miniaturization, which formes the basis of IT development. The main sources of carbon dioxide emissions are energy production, transportation and certain industrial processes. Carbon-neutral techniques already exist in all of these sectors, but they are often too expensive and/or not efficient enough to become widespread.

The various low reduced dimensional nanostructures (0D, 1D, 2D) are highly important elements for the development of new technologies today. Nanostructures with different dimensions are used in different fields of industry, e.g. in catalysis, fuel cells, nanoelectronics, informatics. Two significant advantages of nanostructures with diverse structures are that (I) in this size range, most materials have different physical and chemical properties than in the bulk phase. The well-known example of this is gold, which is almost completely inert in chemical reactions in the bulk phase, while the ~2 nm Au clusters are able to catalyze the oxidation of carbon monoxide at room temperature. (II) The smaller size also implies that smaller quantities can be used to achieve high efficiencies in chemical processes, which results in lower costs. Numerous surface and materials science techniques are available to explore the properties of nanomaterials, either in imaging (electron microscopy and scanning microprobe methods) or in spectroscopy (electron and ion spectroscopies and synchrotron based methods). These measurement methods nowadays can be used to study the structure, chemical environment or binding system of a substance under different conditions (in situ ↔ ex situ, ultra-high vacuum (UHV) ↔ near atmospheric pressure). Due to the high purity available, UHV conditions tend to provide useful information in the study of model systems that contributes to the design of our measurements and experiments at atmospheric pressure, and most importantly, to our understanding of the results.

Real heterogeneous catalysts have a very complex structure, therefore in model catalysis catalytically active metal nanoparticles are prepared on oxide single crystals or ultra-thin oxide single crystal films for a better understanding of the processes taking place on their surface. In the first half of my doctoral dissertation, my goal was to gather information about the

interactions between cobalt and $CeO_2(111)$, how they change as a function of the amount of metal, the change in temperature, and the degree of reduction of cerium. It is known that cerium dioxide-supported cobalt effectively catalyzes the reforming of bioethanol (steam reforming of ethanol), which is a promising pathway for renewable hydrogen production.

Since the discovery of graphene and its unique properties, numerous publications have been published on the subject of 2D nanomaterials. The near-resistance-free electrical and thermal conductivity of graphene has inspired research into similar 2D nanomaterials among semiconductors (MoS2) or insulators (hexagonal BN, h BN). Hexagonal boron-nitride is of particular interest among 2D materials, because it is almost perfectly isomorphic to graphene. While its thermal conductivity does not lag behind significantly, in contrast to graphene, h-BN is electrically insulating. It is well-known from literature that h-BN has a periodically undulating, so called nanomesh morphology on Rh(111) due to the strong metal-nitride interaction and the significant lattice mismatch. Conversely, h-BN forms a nearly planar layer on elements of the copper group due to the weak metal-nitride interaction. In the second half of my studies, I investigated the properties of gold-rhodium and gold/boron-nitride/rhodium systems. I was curious about the growth mechanism of gold on the surface of Rh (111) at different temperatures, what changes take place in the outermost atomic layer as a result of thermal treatments after deposition, and what chemical changes occur in the surface layer in the meantime. I investigated the growth mechanism of gold and the change of its chemical environment on the nanomesh surface of hexagonal boron nitride, as well as the effect of gold intercalation on the electron structure of boron nitride. Furthermore, I investigated the growth of h-BN on Au-Rh alloy surfaces at different gold contents.

In my work, in addition to X-ray photoelectron spectroscopy (XPS), my main experimental method was low-energy ion scattering spectroscopy (LEIS), which provides information about the outermost atomic layer of the surface, when using noble gas ions. Although not common, in some material systems the neutralization probability of the noble gas ions used depends also on the chemical environment of the atom under study (neutralization effect), which makes quantitative analysis difficult. For this reason, during the LEIS measurements, I paid special attention to check these possible effects. XPS studies provided information about the oxidation state of surface layer, while the comparison of XPS and LEIS results revealed diffusion processes perpendicular to the surface.

## 2. <u>Experimental</u>

During my doctoral work, the measurements were performed in a UHV chamber with a base pressure of $\sim 5 \times 10^{-10}$ mbar. The chamber is equipped with a Leybold hemispherical analyser, which can also be used for LEIS, XPS, and Auger electron spectroscopy (AES) measurements. I used a quadrupole mass spectrometer to analyze the residual gas. $He^+$ and $Ne^+$ ions were released to the surface with a kinetic energy of 800 eV and low ion flux ($\sim 30$ nA/cm$^2$) in LEIS experiments. The the scattering angle was 95°. An Al Kα X-ray source was used for XPS measurements. To calibrate the binding energy scale, I used the $4f_{7/2}$ peak (84.0 eV) of a thick (quasi-bulk) Au layer and the $2p_{3/2}$ peak (932.6 eV) of the pure Cu(111) surface for the measurements on the Cu(111) single crystal. For measurements on Rh (111), the Rh $3d_{5/2}$ peak (307.2 eV) was the second calibration point together with Au $4f_{7/2}$. The detection angle was 16° from surface normal.

Surface cleaning of Cu(111) was performed by cycles of $Ar^+$ sputtering at 300 K and annealing at 1000 K in UHV.

A monolayer (ML) oxygen was defined as the surface atomic density of Cu(111) ($1.78 \times 10^{15}$ atoms/cm$^2$). Ce (99.9%) and Co (99.99%) metals were deposited using a commercial 4-pocket PVD source (Oxford Applied Research). A monolayer of $CeO_2$ is defined as an entire $CeO_2$(111) triple layer (i.e., O-Ce-O, $7.87 \times 10^{14}$ Ce atoms/cm$^2$) with a thickness of 3.13 Å. In the case of Ce metal, the monolayer coverage is defined as the surface atomic density of the close packed (0001) surface of the dhcp bulk β phase, because under the conditions I studied it is the thermodynamically stable phase, and therefore 1 ML Ce $\sim 8.53 \times 10^{14}$ atoms/cm$^2$ [1]. By definition, Co coverage is 1 ML if the surface concentration of Co atoms is equal to the surface atomic density of Co(0001) ($1.8 \times 10^{15}$ atoms/cm$^2$). The evaporation rate of Ce and Co was determined with a quartz crystal microbalance (QCM), which was 0.07 ML/min for Ce and $CeO_2$, while that of cobalt was 0.5 ML/min.

Cleaning of the Rh(111) single crystal (dia. 6 mm×1.5 mm, orientation accuracy: 0.1°) was performed in cycles of $Ar^+$ sputtering at 300 K and annealing at 1200K in UHV. After the last cycle, I heated the sample at 1050 K in $\sim 3 \times 10^{-8}$ mbar $O_2$ for 30 minutes, then cooled it down below 350 K in an oxygen atmosphere. The final step of sample preparation was a 1200 K and 1 minute heating in UHV. The h BN monolayer was prepared by thermal decomposition of > 99.8% pure borazine (Katchem Ltd.) at 1000 K. For the deposition of Au, I used high purity (99.95%) gold in the evaporator mentioned above. Gold coverage is defined by the surface atomic density of Rh(111) (1 ML $\sim 1.60 \times 10^{15}$ atoms/cm$^2$). I use this definition, because the

growth of gold is pseudomorphic until 1 ML on Rh(111) surface [2]. The evaporation rate of gold was 0.2 ML/min.

# 3. Presentation of new scientific results

### 1. Neutralization effects in the Ce–O–Cu terner system

1.1. In the LEIS study of oxygen adsorption on Cu (111), a signal attributable to oxygen was naturally only detectable in spectra recorded with helium, since the mass of neon exceeds that of oxygen. As $O_2$ exposure was increased, in addition to the increase in the intensity of the oxygen signal obtained with helium, the intensity of Cu signal decreased in both the helium and neon spectra, showing a linear relationship between them. Based on the linear relationship between the intensity changes of copper and oxygen signals, we showed that the adsorption of $O_2$ on Cu(111) does not induce a neutralization effect either with helium or neon.

1.2. Monitoring the deposition of Ce with LEIS, we found a linear relationship between the intensity changes of cerium and copper signals recorded with $He^+$ ions, i.e. no neutralization effects occurs for $He^+$ ions during the deposition of cerium on Cu(111). In spectra recorded with $Ne^+$ ions, the correlation between the intensity changes of Ce and Cu peaks was not linear. However, when the copper signal intensities recorded with helium were compared to those obtained with neon, a linear correlation was found between them. Thus, we validated that cerium induces a significant matrix effect for $Ne^+$ ions, so only measurements with helium, and the Cu intensity recorded with neon can be used for quantitative analysis.

1.3. Comparing the LEIS intensity values obtained with helium in the study of cerium dioxide formation on Cu(111), the total surface fraction of copper and oxygen decreased linearly with increasing cerium intensity, thus proving that no matrix effects arise for helium. Comparing the Ce intensities measured with neon with the values recorded with helium, we also found a linear relationship, so in the case of cerium-dioxide there are no neutralization effects for neon either. We have demonstrated that the relative sensitivity factors of helium LEIS determined separately during oxygen adsorption and metal cerium deposition can also be used for the quantitative characterization of $CeO_2$ growth.

## 2. Investigation of the growth mechanism of Ce and CeO$_2$ on Cu(111)

2.1. We proved that cerium grows two-dimensionally on Cu(111) up to 0.5 ML, above which the growth is three-dimensional. Complete coverage of the surface can be reached with 2.0 ML Ce. Based on the results of subsequent oxygen adsorption measurements on Ce deposits, we found that cerium wetted the surface less in this case, in other words, the average height of cerium clusters increased as a result of oxygen adsorption.

2.2. During CeO$_2$ synthesis, I investigated the effect of O$_2$ pressure on the continuity and stoichiometry of the oxide film. When cerium was deposited in $3\times10^{-6}$ mbar of oxygen, the 16 ML ceria film was basically continuous and only 2% of cerium was reduced (Ce$^{3+}$), but ~0.015 ML of copper also appeared in the topmost atomic layer. Conversely, synthesizing CeO$_2$ in $5\times10^{-7}$ mbar of oxygen reduced the amount of surface Cu to ~0.003 ML, implying that the 16 ML oxide film was continuous, but the proportion of Ce$^{3+}$ ions increased to 4%.

## 3. Investigation of the interaction of Co and CeO$_2$

3.1. Based on LEIS results, the growth of cobalt was found to be two-dimensional on CeO$_2$(111) up to 0.3 ML coverage, whereas larger amounts of Co form 3D clusters on ceria. Neither cobalt nor cerium signals are affected by neutralization matrix effects in LEIS, independent of whether helium or neon is used. This finding is supported by the linear relationships observed in the comparison of the respective intensity data. However, upon the deposition of Co, a significant deviation from the linear behavior was observed in the intensity of the O LEIS peak. Examining the adsorption of O$_2$ on a quasi-bulk, continuous cobalt film, we found a significant neutralization effect with He$^+$ ions for oxygen.

3.2. XPS measurements revealed that Co was oxidized to Co$^{2+}$ up to a coverage of 0.2 ML on the surface of ceria during deposition, while partially reducing it. At higher amounts of cobalt, a gradual increase in the proportion of metallic cobalt was observed, leading us to assume that the oxidation of cobalt during deposition is limited to the Co–CeO$_2$ interface. In addition, reduction of an increasing fraction of Ce$^{4+}$ ions to Ce$^{3+}$ was detected during deposition.

3.3. As a result of thermal treatments, increasing oxidation of cobalt and diffusion of Co$^{2+}$ ions into the deeper layers of the CeO$_2$ film were observed.

3.4. Evaporation of cobalt to a reduced CeO$_x$ layer showed that the redox reaction between cobalt and CeOx was more limited during deposition, i.e., cobalt was less oxidized and

the $Ce^{3+}/Ce^{4+}$ ratio changed to a smaller extent than on stoichiometric $CeO_2$. This limited redox reaction also hindered the diffusion of cobalt into deeper layers during heat treatments.

## 4.   Study of gold growth on Rh(111)

4.1. Based on LEIS data, we proved that gold forms two-dimensional clusters up to 0.5 ML on the surface of Rh(111) at 500 K, while larger amounts of Au stabilized on the surface in 3D clusters. For a complete coverage of rhodium~2.5 ML of gold is required.

4.2. With LEIS, we examined the growth of Au on Rh(111) at different substrate temperatures, and there was no detectable change in the sticking coefficient of gold in the temperature range between 500 K and 700 K, so it is considered unity at these temperatures.

4.3. Based on LEIS measurements, gold wets the rhodium surface better at 700 K than at 500 K, especially in the 1-3 ML range; nevertheless the growth of Au is 3D above 0.5 ML at both temperatures. Therefore, we hypothesize that the deviation from 2D growth at 500 K has kinetic rather than thermodynamic reasons. The better wetting experienced at 700 K may also be partly due to surface alloying.

## 5.   Investigation of the interaction between Au and h-BN on Rh(111)

5.1. The h-BN film prepared by the decomposition of borazine at 1000 K was nearly perfectly continuous, because at the end of the synthesis, the contribution of the Rh signal in the LEIS spectrum, was below the detection limit, which is 0.0005 ML rhodium equivalent. h-BN induced no neutralization effects on the rhodium signal using either $He^+$ or $Ne^+$ ions.

5.2. Gold forms 2D clusters on the surface of h-BN nanomesh up to 0.1-0.2 ML, while at higher Au coverages the growth is clearly 3D.

5.3. During the heating of the gold clusters deposited on the h-BN/Rh(111) surface, we observed a continuous decrease in gold intensity in LEIS spectra up to 700 K, indicating Ostwald ripening, intercalation and/or desorption. However, based on XPS measurements with the same amounts of gold, desorption is not significant up to 700 K. In the temperature range of 700–1050 K, the intensity of Au in the LEIS spectra gradually decreased below the detection limit, implying complete intercalation and/or desorption of gold. The peak area of the Au 4f region up to 1050 K decreased to 75% of its initial value, hence the extent of desorption is limited, and the majority of gold intercalated. At temperatures above 1050 K, the h-BN film gradually loses its continuity and Rh as well as Au reappear in LEIS spectra.

**6. Synthesis of h-BN on Au-Rh alloy surfaces**

6.1. We have shown that on the Au-Rh surface alloy formed on Rh(111), the Rh LEIS signal disappears at much lower borazine exposure than the gold peak. This is due to the stronger interaction between Rh and borazine (and fragments thereof) and the higher activity of Rh in the decomposition of borazine.

6.2. We have shown that as the amount of gold on the alloyed surface increases the decrease in the Au signal becomes increasingly slower. The decrease in the gold signal is caused by the diffusion of borazine/boron-nitride fragments formed on rhodium onto gold, the efficiency of which decreases as the number of surface Rh atoms decreases.

6.3. We have shown that in h-BN synthesis measurements on the surface alloy, after the disappearance of the LEIS rhodium signal, the Au signal decreased further upon further borazine exposures; and this attenuation was much steeper than in measurements made on a continuous (~ 4 ML) gold film. The explanation of the observed behavior, in accordance with point 6.2, is that fragments of borazine/boron nitride adsorbed on Rh atoms migrate to Au atoms, thus accelerating the coating of gold by h-BN. This way some Rh atoms get uncovered for short time, but these will be covered instantaneously by borazine molecules and their decomposition products, therefore Rh LEIS intensity stays zero.

# 4. Publications forming the basis of the dissertation

1. **G. Vári**, L. Óvári, J. Kiss, Z. Kónya

   *LEIS and XPS investigation into the growth of cerium and cerium dioxide on Cu(111)*

       Phys. Chem. Chem  Phys. **17** (7). pp. 5124-5132. (2015)

       MTMT: [2811919]

         **IF: 4,449**

2. **G. Vári**, L. Óvári, C. Papp, H-P. Steinrück, J. Kiss, Z. Kónya

   *The Interaction of Cobalt with $CeO_2(111)$ Prepared on Cu(111)*

       J. Phys. Chem. C **119:**(17) pp. 9324-9333. (2015)

       MTMT: [2881646]

         **IF: 4,509**

3. L. Óvári, A. Berkó, **G. Vári**, R. Gubó, A. P. Farkas, Z. Kónya

   *The growth and thermal properties of Au deposited on Rh(111): formation of ordered surface alloy.*

       Phys. Chem. Chem  Phys. **18** pp. 25230-25240. (2016)

       MTMT: [3101262]

         **IF: 4,123**

4. R. Gubó, **G. Vári**, J. Kiss, A. Farkas, L. Óvári, A. Berkó, Z. Kónya

   *Tailoring the hexagonal boron nitride nanomesh on Rh(111) by gold*

       Phys. Chem. Chem. Phys. **20** pp. 15473-15485. (2018)

       MTMT: [3368595]

         **IF: 3,567**

         **ΣIF: 16,648**

# 5. Other publications

1. A. Sápi, Gy. Halasi, J. Kiss, D. G. Dobó, K. L. Juhász, V. J. Kolcsár, Zs. Ferencz, **G. Vári**, V. Matolin, A. Erdőhelyi, Á. Kukovecz, Z. Kónya

   *Supporting Information for - In-situ DRIFTS and NAP-XPS exploration of the complexity of $CO_2$ hydrogenation over size controlled Pt nanoparticles supported on mesoporous NiO*

   > J. Phys. Chem. C **122** pp. 5553-5565. (2018)
   > MTMT: [3339431]

                                                                                    **IF: 4,309**

2. Palotás Krisztián, Óvári László, **Vári Gábor**, Gubó Richárd, Farkas Arnold P, Kiss János, Berkó András, Kónya Zoltán

   *Au–Rh Surface Structures on Rh(111): DFT Insights into the Formation of an Ordered Surface Alloy*

   > J. Phys. Chem. C **122** pp. 22435-22447. (2018)

   > MTMT: [3422662]

                                                                                    **IF: 4,309**

3. Farkas Arnold Péter, Szitás Ádám, **Vári Gábor**, Gubó Richárd, Óvári László, Berkó András, Kiss János, Kónya Zoltán

   *Effect of Gold on the Adsorption Properties of Acetaldehyde on Clean and h-BN Covered Rh(111) Surface*

   > Top. Catal. **61** pp. 1247-1256. (2018)

   > MTMT: [3370969]

                                                                                    **IF: 2,321**
                                                                                    **ΣIF: 10,939**

**ΣΣIF: 27,587**

# 6. Conference participation

1. **Vári G.**, Óvári L., Kiss J., Kónya Z.

   CeO$_2$(111) felületen létrehozott modellkatalizátorok spektroszkópiai vizsgálata

   *I. Innováció a Természettudományban – Doktorandusz Konferencia*

   Szeged (Hungary), 2014. **oral**

2. **G. Vári**, L. Óvári, J. Kiss, Z. Kónya

   Spectroscopic investigation into the interaction of Co with CeO$_2$(111)

   *15$^{th}$ Joint Vacuum Conference*

   Bécs (Ausztria), 2014. **oral**

3. **Vári G.**, Óvári L., Kiss J., Kónya Z.

   CeO$_2$(111) felületen létrehozott modellkatalizátorok spektroszkópiai vizsgálata

   *MTA Felületkémiai és Nanoszerkezeti Munkabizottsági ülés*

   Budapest (Hungary), 2014. **oral**

4. L. Óvári, **G. Vári**, S. Krick-Calderon, Z. Kónya, J. Kiss, C. Papp, H.- P. Steinrück

   Characterization of a Co/CeO$_2$(111) model catalyst and its interaction with ethanol near ambient pressure

   *Berlin Rideal Conference*

   Berlin (Germany), 2015. **poster**

5. **G. Vári**, L. Óvári, C. Papp, H.-P. Steinrück, J. Kiss, Z. Kónya

   Growth and thermal effects of Co on CeO$_2$(111)

   *31$^{st}$ European Conference on Surface Science*

   Barcelona (Spain), 2015. **poster**

6. L. Óvári, A. Berkó, R. Gubó, **G. Vári**, J. Kiss, A. P. Farkas, Z. Kónya

   Gold on hexagonal boron nitride nanomesh prepared on Rh(111): Growth and intercalation

   *16th Joint Vacuum Conference*

   Portoroz (Slovenia), 2016. **oral**

7. L. Óvári, A. Berkó, R. Gubó, **G. Vári**, J. Kiss, A. P. Farkas, Z. Kónya

   Growth and intercalation of gold on hexagonal boron nitride nanomesh prepared on Rh(111)

   *20th International Vacuum Congress*

   Busan (South Korea), 2016. **oral**

8. A. Berkó, L. Óvári, A. P. Farkas, R. Gubó, **G. Vári**, J. Kiss, Z. Kónya

Formation of Au-Rh surface alloy and the effect of Au on the structure of h-BN film grown on Rh(111) surface

*32$^{nd}$ European Conference on Surface Science*

Grenoble (France), 2016. **oral**

9.  A. P. Farkas, D. Jurdi, R. Gubó, **G. Vári,** L. Óvári, A. Berkó, J. Kiss, Z. Kónya

    Adsorption properties of ethanol on gold decorated h-BN nanomesh prepared on Rh(111) surface

    *32$^{nd}$ European Conference on Surface Science*

    Grenoble (France), 2016. **poster**

10. **G. Vári**, R. Gubó, J. Kiss, A. P. Farkas, L. Óvári, A. Berkó, Z. Kónya

    Interaction of gold with the hexagonal boron nitride nanomesh prepared on Rh(111)

    *7$^{th}$ Szeged International Workshop on Advances in Nanoscience*

    Szeged (Hungary), 2016. **oral**

11. **Vári G.**, Gubó R., Farkas A. P., Óvári L., Kiss J., Berkó A., Kónya Z.

    Arany növekedése és interkalációja Rh(111)-en növesztett h-BN nanohálón

    *MTA Felületkémiai és Nanoszerkezeti Munkabizottsági ülés*

    Budapest (Hungary), 2016. **oral**

12. **G. Vári**, R. Gubó, J. Kiss, A. Farkas, L. Óvári, A. Berkó, Z. Kónya

    Interaction of Au, Rh and Au-Rh alloys with the Hexagonal Boron Nitride monolayer studied on Rh(111)

    *33$^{rd}$ European Conference on Surface Science*

    Szeged (Hungary), 2017. **poster**

13. A. P.Farkas, Á. Szitás, **G. Vári**, L. Óvári, A. Berkó, J. Kiss, Z. Kónya

    Effect of gold on the adsorption properties of acetaldehyde on clean and h-BN covered Rh(111) surface

    *33$^{rd}$ European Conference on Surface Science*

    Szeged (Hungary), 2017. **oral**

14. **Gábor Vári**, Richárd Gubó, János Kiss, Arnold Farkas, László Óvári, András Berkó, Zoltán Kónya

    Interaction of Au and Rh with a Hexagonal Boron Nitride monolayer studied on Rh(111)

    *17$^{th}$ Joint Vacuum Conference*

    Olomouc (Czech Republic), 2018. **poster**

15. **Gábor Vári**, Richárd Gubó, János Kiss, Arnold Farkas, László Óvári, András Berkó, Zoltán Kónya

    Interaction of Au, Rh and Au-Rh alloys with the Hexagonal Boron Nitride monolayer studied on Rh(111)

    *8th Szeged International Workshop on Advences in Nanoscience*

    Szeged (Hungary), 2018. **poster**

16. **Vári Gábor**, Gubó Richárd, Kiss János, Farkas Arnold, Palotás Krisztián, Óvári László, Berkó András, Kónya Zoltán.

    Rh(111) felületen létrehozott hexagonális bórnitrid nanoháló kölcsönhatása fémekkel

    *Magyar Fizikus Vándorgyűlés 2019*

    Sopron (Hungary) 2019. **oral**

17. **Vári Gábor**, Kiss János, Farkas Arnold, Palotás Krisztián, Óvári László, Berkó András, Kónya Zoltán

    Rh(111) felületen létrehozott hexagonális bórnitrid nanoháló kölcsönhatása fémekkel

    *MTA Felületkémiai és Nanoszerkezeti Munkabizottsági ülés*

    Online, 2020. **oral**

18. **Gábor Vári**, Richárd Gubó, János Kiss, Arnold Farkas, László Óvári, András Berkó, Zoltán Kónya

    Intercalation of Au on hexagonal boron nitride monolayer prepared on Rh(111) and on gold coated Rh(111)

    *18th International Conference on Thin Films and 18th Joint Vacuum Conference*

    Online, 2020. **poster**

## 7. <u>References</u>

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[2]    L. Óvári, A. Berkó, G. Vári, R. Gubó, A.P. Farkas, Z. Kónya, Phys. Chem. Chem. Phys. 18 (2016) 25230–25240. https://doi.org/10.1039/C6CP02128J.