STAND-ALONE PROJECT

FINAL REPORT

Project number	**P27649-N20**
Project title[1]	**Quantifying photoemission of organic molecular films**
	German title: Photoemission von organischen Molekülfilmen
Project leader	**Assoz.-Prof. Dipl.-Ing. Dr. Peter PUSCHNIG**
Project website[2]	**http://physik.uni-graz.at/~pep/P27649-N20/index.html**

[1] Short title in English and German language
[2] Projects that started after January 1, 2009 are encouraged to have a website.

I. Summary for public relations work

1. Zusammenfassung für die Öffentlichkeitsarbeit

Albert Einstein hat seinen Nobelpreis nicht für die Entwicklung der Relativitätstheorie erhalten, sondern für seine Erklärung des photoelektrischen Effekts. Darunter versteht man den Prozess, bei dem Lichtteilchen (Photonen) Elektronen aus einer Oberfläche herauslösen. Heutzutage wird der photoelektrische Effekt dazu verwendet, um die Elektronenzustände in neuartigen Materialien zu untersuchen. Dabei wird die Materialprobe, die sich in einer Vakuumkammer befindet, mit ultraviolettem Licht bestrahlt, und die herausgelösten Elektronen werden in Bezug auf ihre kinetische Energie und Emissionsrichtung detektiert. Dieses Verfahren bezeichnet man als winkelaufgelöste Photoemissionsspektroskopie, oder mit der englischen Bezeichnung als *angle-resolved photoelectron spectroscopy* (ARPES). Gegenstand dieses Forschungsprojekts war nun die die theoretische Beschreibung der ARPES basierend auf quantenmechanischen Prinzipien.

Im Rahmen dieses Projekts wurde gezeigt, dass sich die Winkelverteilung der emittierten Elektronen unter gewissen vereinfachenden Annahmen sehr einfach interpretieren lässt, und damit sehr tiefgreifende Rückschlüsse auf die quantenmechanischen Zustände der Elektronen an der Oberfläche der Materialprobe erlaubt. Dieses als Photoemissions-Tomographie bezeichnete Verfahren erlaubte etwa erstmals dreidimensionale Bilder der quantenmechanischen Elektronenwellenfunktion (Orbital) von organischen Molekülen aus den ARPES Messdaten zu rekonstruieren. Dies ermöglicht etwa die detaillierte Untersuchung der Wechselwirkungen zwischen Molekül und Substrat und gibt Aufschluss darüber, welche Molekülzustände an der elektronischen Ankopplung von Molekül zu Trägermaterial beteiligt sind. Diese und ähnliche Fragen sind nicht nur von grundlegender Bedeutung. Sie ermöglichen in weiterer Folge auch die Untersuchung vieler physikalischer und chemischer Prozesse an der Grenzfläche zwischen Molekülen und Oberflächen. Beispiele bilden das Maßschneidern von katalytischen Oberflächen, Sensoren, neuartigen Molekülen und Nanostrukturen aus dem Bereich Energiegewinnung, etwa Photovoltaik, und Energiespeicherung, aber auch die Identifizierung und Charakterisierung unbekannter Moleküle. Darüber hinaus liefert die Photoemissions-Tomographie auch wertvolle experimentelle Daten, die bei der Weiterentwicklung von quantenchemischen Berechnungsverfahren als „Benchmark“ dienen können.

2. Summary for public relations work

Albert Einstein has received his Nobel Prize in physics not for his development of relativity theory, but for the explanation of the photoelectric effect. This is a process in which a light particle (photon) incident on a material kicks out an electron from the surface of the material. Nowadays this photoelectric effect is used to study the electronic states in novel materials and interfaces. Thereby, the material under investigation, which is situated in a vacuum chamber, is irradiated with ultraviolet light and the emitted electrons are detected in terms of their kinetic energy and their emission direction. This experimental method is known as angle-resolved photoemission spectroscopy (ARPES). The theoretical characterization of ARPES based on a quantum mechanical description was the topic of this research project.

In the framework of this project, it has been shown that – under certain simplifying assumptions – the angular distribution of the emitted electrons finds a simple and intuitive interpretation and allows for profound conclusions about the quantum mechanical electron states at the surface of the material under investigation. This technique, which we termed photoemission tomography, has, for instance, enabled to reconstruct three-dimensional images of quantum mechanical wave functions of electrons (orbitals) of molecules adsorbed on surfaces from ARPES experiments. This facilitates a detailed investigation of the interactions between molecules and the underlying substrate and sheds light on the question which molecular states are mainly responsible for the coupling to the substrate. Such problems are not only of fundamental interest, but they also allow for the analysis of many physical and chemical processes which take place at the interface between molecules and surfaces. Examples include identification and characterization of novel molecules and nanostructures or the tailoring of catalytic surfaces, sensors, or novel molecules and nanostructures to be used as energy harvesting materials, e.g. as photovoltaic or energy storage materials. Moreover, photoemission tomography yields valuable and rich experimental data which can be used as benchmark to guide the further development of quantum mechanical electronic structure methods for solving the complicated many-electron Schrödinger equation.

II. Brief project report

1. Report on research work

1.1 Information on the development of the research project

When starting the project in February 2015, a renaissance of angle-dependent photoemission spectroscopy (ARPES) in the field of organic electronics could be observed. This was, at least partly, motivated by observations that a plane wave approximation for the final state provided a qualitatively correct, and yet simple and intuitive, description of the transition matrix element in terms of the Fourier transform of the initial state orbital [Puschnig et al., Science 326, 702 (2009)]. Nevertheless, it became clear that there are certainly limitations of the plane wave approximation for the final state [Bradshaw and Woodruff, New Journal of Physics 17, 013033 (2015)]. This situation has led to the overall project goal of achieving a fully quantitative description of the photoemission cross section of organic molecular films. In particular, three aspects to reach this aim have been formulated in the proposal:

(i) Investigate what role the level of theory, at which the initial state energies and wave functions are treated, plays for photoemission cross section

(ii) Examine how final state scattering can be incorporated into the theoretical description and test its role on actual photoemission angular distributions

(iii) Explore the influence of the polarization of the incident light on the photoemission cross section, for instance, the circular dichroism in the angular distribution (CDAD) of photoemitted electrons.

As outlined in detail in Section 1.2, all research goals have indeed been tackled in the course of the project and important advancements could be achieved as documented by a number of peer-reviewed publications [1–19]. It should be mentioned that some research directions have not been envisioned in 2014, such as the application of photoemission tomography (PT) to molecules on thin dielectric layers [12] or the application of PT to extended 2D layers [1,11,14]. Nevertheless, these results contributed successfully to the research goals of the current project. On the other hand, some of the planned research endeavours, e.g. a yet more advanced theoretical description beyond the plane wave final state, are still ongoing and have flown into the joint experimental and theoretical follow-up project “Exploring the foundations of photoemission tomography” (international project I3731 funded by FWF and DFG).

1.2 Most important results and brief description of their significance (main points) with regard to the following:

Contribution to the advancement of the field. The results obtained in the course of this project have contributed to establishing photoemission tomography (PT) as a new experimental window to the structural and electronic properties of thin (organic) layers on surfaces. PT has helped to extract layer-resolved electronic and geometric information [4], contributed to clarify the charge state and/or charge transfer due to doping or across dielectric layers [6,12,13,17,18], revealed symmetry breaking upon electron transfer into molecules [8,15], and its theoretical description has been extended to extended 2D layers [1,11,14]. It should also be regarded as a success of the project that other groups have been pursuing the PT technique. For instance, a more robust phase retrieval algorithm has been presented [Kliuiev et al. PRB 98, 085426 (2018)], a real-time density functional theory approach to photoemission has been developed [Dauth et al. Phys. Rev. Lett. 117, 183001

(2016); Wopperer et al. The European Physical Journal B 90, 51 (2017)], and a multi-scattering approach has been implemented molecules in the gas phase [Komiya at al. J. Electr. Spectr. Rel. Phenom. 220, 21 (2017)].

Breaking of new scientific / scholarly ground. One major result of the project regards the extension of PT to *photon energy dependent* measurements. During the project, it became clear that the acquisition of quantitatively reliable experimental angle-resolved photoemission data is a non-trivial task and requires special measures concerning the normalization of the data. Note for instance, that the preliminary photon energy dependence shown in Fig. 2 of the proposal turned out to be wrong due to problems in normalization. It is worth noting that the finally published results [3,B1] have demonstrated that the plane wave final state (PWFS) description turned out to be in better agreement with experimental observations than initially thought. Particularly, the PWFS accounts well for the overall dependence of the photocurrent on the photon energy which has allowed us to reconstruct three-dimensional real space images of orbitals from experimental data. There are, however, additional modulations in the photon energy dependence which we have ascribed to final state scattering effects which will be explored in more detail and for series of molecule / substrate combinations in the follow-up project (I 3731).
Another breakthrough has been achieved by generalizing the theoretical description of PT transition matrix elements from isolated molecule initial states to *extended two-dimensional layers interacting with a substrate*. First, the band dispersion of initial states has been allowed for and, for instance applied to free-standing graphene layers [1]. In a second step, also the interaction with the substrate has been taken into account [14] which has allowed to include (substrate)-enhanced intermolecular dispersions. It is important to note that we have also generalized the final state of the photoemission by incorporating an empirical damping factor [14], [Moser J. Elec. Spectr. Rel. Phenom. **214**, 29-52 (2017)]. While this approach does not take into account scattering effects in the final state, it can be regarded as a step in the right direction: It captures the experimentally known free-mean path of the photoemitted electrons and it introduces a chirality, thereby leading to a circular dichroism effect in the angular emission patterns which can, at least, partly explain experimental observations [Yang et al., in preparation].
As a third important outcome of the project, we have demonstrated that PT is able to provide an orbital-by-orbital characterization of organic molecular films, thereby creating a compelling benchmark for ab initio electronic structure theory [10]. This is because, from a theoretical point of view, the photoelectron angular distribution (PAD) is quite robust when varying exchange-correlation functionals within DFT or even when switching to wave-function based post Hartree-Fock methods. Thereby, the PAD can be used to decompose experimental data into individual molecular orbitals contributions which in turn can be used to challenge ab-initio theories in terms of the energy alignment and ordering of single particle excitation energies [10].

Most important hypotheses / research questions developed. At the start of the project, Bradshaw and Woodruff have published their paper “Molecular orbital tomography for adsorbed molecules: is a correct description of the final state really unimportant?” [New Journal of Physics 17, 013033 (2015)]. In their paper, Bradshaw and Woodruff provide a detailed critique of the plane-wave final state description and high-light situations in which the photoemission tomography approach is likely to lead to major errors, and they propose test experiments that could provide clear information on the extent of these problems. Some of those propositions have flown into the follow-up project since their detailed analysis required

a concerted effort of theory and experiment. However, some hypotheses could already been tested in this project. In particular, it was found in our recent paper “Can photoemission tomography be useful for small, strongly-interacting adsorbate systems?” [19] that PT with a plane-wave final state description may also give useful insights for smaller organic molecules (such as benzene) on a more-interacting substrates (such as Palladium). However, this work has also clearly demonstrated the limitations of the PWFS description and will be the starting point for further investigations and theoretical developments.
A result which has also not been anticipated from the beginning is that PT can be used to quantify the amount of charge transferred to organic molecules from metal surfaces through thin insulating layers [12]. With the help of calculated photoemission cross-sections, it was possible to unambiguously conclude from experimental data that pentacene adsorbed on two layers of MgO / Ag(100) gets singly charged leading to single occupied molecular orbital (SOMO). This result [12] has triggered a whole series of systematic studies of various organic molecules (pentacene, sexi-pheynl, porphyrines, PTCDA) on metals covered by insulating layers of various thicknesses. The results of these studies are currently being summarized in a manuscript [P. Hurdax et al.] and provide deep insights into the mechanisms governing charge transfer process across dielectric layers.

The following new methods / tools have been developed. (i) The initial state description has been generalized to Bloch states thereby allowing for the description of extended 2D-layers interacting with a substrate [1,14]. (ii) The final state description has been modified to include an empirical, exponential damping term [14]. This takes into account the free-mean path of photoelectrons and introduces a circular dichroism in the angular distribution. (iii) A Python-based tool for easy analysis of the PAD of organic molecules has been developed. Currently, this program code with a graphical user interface allowing also the processing of experimental data is in a beta test stage and available to the project partners of the follow-up I 3731 project, but will be made available to the public in future. (iv) In the course of the project, a python-based data base containing all relevant data characterizing the gas phase electronic structure of organic molecules has been created. It can be browsed with a web-browser and, currently, the data base contains about 50 typical pi-conjugated organic molecules that have been calculated with four different exchange-correlation functionals: PBE-GGA, B3LYP, HSE and a per-system optimally tuned range-separated hybrid (OT-RSH). Exemplary results from the data based have been published in [16]. Apart from the orbital energies, this data base also allows easy access to real- and momentum space representations of the molecular orbitals and thereby simulations of the photoelectron angular distributions. Currently, the database is available to the project consortium of the follow-up project I 3731, but it is planned to make this database publically available on the web which will help to further promote the photoemission tomography technique.

Relevance for other (related) areas of science. In particular, the capability to reconstruct images of molecular orbitals from the experimental photoemission data has challenged common sense of the physics and chemistry research communities. For instance, the question of how to interpret the orbitals reconstructed from the experimental ARPES data has stimulated many discussions at scientific conferences. In this context, it is also worth mentioning that we have been invited to contribute a paper to the physics-education journal “Physik in unserer Zeit” entitled “Elektronenorbitale in 3D - Photoelektronen-tomographische Bilder von Molekülorbitalen” [B1]. In this paper (in German language) we attempted to explain the PT technique for a broader audience.

1.3 Information on the execution of the project, use of available funds and (where appropriate) any changes to the original project plan relating to the following:

Duration. The project has been started in February 2015 and has ended on 31st of December 2018.

Use of personnel. Bernd Kollmann has been employed as a PhD student from June 2015 to December 2018, Daniel Lüftner has been employed as a PostDoc from June 2015 to August 2018 with a four-month interruption due to a parental leave. Towards the end of the project (April – August 2018) Mathias Schwendt has been employed as a PhD student who is continuing his PhD in the follow-up project I 3731.

No equipment was purchased.

No significant deviation from the original project plan.

2. Personnel development – Importance of the project for the research careers of those involved (including the project leader)

Peter Puschnig. The project's output, including scientific publications, invitations to conference and seminar talks, education of Master and PhD students, is an important aspect in the qualification process of the PI which involves an evaluation every six years (the next evaluation will be in 2020).
Daniel Lüftner has advanced his scientific career as a PostDoc by high-rank publications and invitations to conferences. For personal reasons, however, he has decided to leave academia and switch to industrial research where he immediately found a position in September 2018.
As a PhD student, **Bernd Kollmann** has been trained in state-of-the electronic structure methods. Moreover, he has gained international experience, for instance, through a research visit at the renowned Weizmann Institute of Science, Rehovot, Israel or through various conference participations where he presented his research results. His main career achievement will be the doctoral degree which will be accomplished in spring 2019.
Mathias Schwendt has entered the project towards the end as a PhD student and has quickly learned the necessary methodology. This has opened his track into the follow-up project I3731, where he is currently employed as a PhD student.
Jana Fuchsberger, **Christian Kern**, **Martin Unzog** and **Oskar Schweighofer** have been involved as Master Students in the project. In the course of their master projects, they have successfully contributed to some of the project's research goals and they already had the chance to present their results as poster contributions at international conferences. Jana has continued her scientific career as PhD student in another research group at the KFU Graz, while Christian Kern is employed as a PhD student in the follow-up project I 3731. Martin Unzog and Oskar Schweighofer are currently finishing their master projects.

It should be noted that apart from the PI's own research group (Lüftner, Kollmann, Schwendt, Kern, Fuchsberger, Unzog, Schweighofer), also PhD students of the experimental collaborators from Graz (Mike Ramsey's group) and Jülich (F. Stefan Tautz's group) have been heavily involved in the project. The scientific exchange between the theoretically oriented and the experimentally oriented research teams has been mutually inspiring and certainly was beneficial for the careers of all involved personnel.

3. Effects of the project beyond the scientific field

On several occasions, project publications have been accompanied by press releases and have been covered in media:

October 5th 2015: Grazer Physiker messen Elektronen-Orbitale in 3-D.
https://steiermark.orf.at/news/stories/2735264/

https://nawi.uni-graz.at/de/neuigkeiten/detail/article/das-unsichtbare-sichtbar-machen-2/

October 5th 2015: Grazer Physiker gewähren atomare Einblicke in 3D (Austrian Press Agency)
https://science.apa.at/rubrik/natur_und_technik/Grazer_Physiker_gewaehren_atomare_Einblicke_in_3D/SCI_20151005_SCI39391351425880628

October 14th 2015: Das Unsichtbare sichtbar machen: Forscher messen Elektronenorbitale von Molekülen in 3D (chemie.de)
http://www.chemie.de/news/155010/das-unsichtbare-sichtbar-machen-forscher-messen-elektronenorbitale-von-molekuelen-in-3d.html

August 25th 2017: Molekulare Allrounder: Porphyrine als organische Halbleiter im Visier.
http://science.apa.at
https://science.apa.at/site/home/login-memberbereich.html?login_required=1&target=natur_und_technik/detail.html?key=SCI_20170825_SCI39391351437767922

http://www.fz-juelich.de/SharedDocs/Meldungen/PGI/PGI-6/EN/2017/2017-08-25-Multi-orbital-charge.html;jsessionid=D49ED6D59D9A8C10DEC56DBF99324538?nn=448936

https://news.uni-graz.at/de/detail/article/molekulare-alleskoenner/

August 27th 2017: Porphyrine könnten Potenzial für organische Halbleiter haben (derStandard.at)
https://derstandard.at/2000063181794/Porphyrine-koennten-Potenzial-fuer-organische-Halbleiter-haben

4. Other important aspects (examples)

Selected conference participations
(A full list is available online: http://physik.uni-graz.at/~pep/P27649-N20/publications.html)

03/2015	Peter Puschnig (invited talk) DPG meeting, TU Berlin, March 15th - 20th, 2015. "Orbital tomography: beyond the plane wave final state approximation"
04/2016	Puschnig, Peter (invited talk) PLESI 2016 (Prospects and Limitations of Electronic Structure Imaging by Angle Resolved Photoemission Spectroscopy), Dresden. 28.04.2016. "Photoemission Tomography: Fundamentals and Applications to Oriented Organic Layers"
11/2016	Daniel Lüftner (invited talk) ASOMEA 8 (Advanced Spectroscopy of Organic Materials for Electronic Applications), Okazaki, Japan, 23.11.2016. "Photoemission Tomography of Ni-TPP on Cu(100)"

03/2017 Peter Puschnig
Jahrestagung der DPG, Dresden, March 22nd, 2017.
"Photoemission Tomography for Extended 2D Layers: The Role of Molecule/Substrate Interactions"

03/2018 Puschnig, Peter
Frühjahrstagung der DPG - Sektion Kondensierte Materie, Berlin, 13.3.2018.
"Identifying on-surface reaction products and orbital modifications with photoemission tomography."

In the framework of the international follow-up project I3731 (“Exploring the foundations of photoemission tomography”), the following workshop will be organized.

Title: “Photoemission Tomography: Applications and Future Developments”
Format: 3-day workshop with 18 invited speakers
Organizers: Peter Puschnig, F. Stefan Tautz, Mathias Richter
Planned Date and Place: Physikzentrum Bad Honnef, 7.-9. Dezember 2020.

The major aim of the above-mentioned seminar will be to set photoemission tomography on firm grounds and to identify the directions of a conceptually more correct description of the photoemission process. The proposed seminar will bring together scientists involved in the experimental and theoretical research into the electronic properties of molecular and 2D materials using momentum space imaging photoemission spectroscopy in the tomographic approach.

III. Attachments

(lists may be as long as required)

1. Scholarly / scientific publications

Publications may only be listed if they relate directly to the project. **Up to three of the most important publications** should be highlighted as such (e.g. printed in bold letters).

1.1 Peer-reviewed publications / already published (journals, monographs, anthologies, contributions to anthologies, proceedings, research data, etc.)

[1] Peter Puschnig, Daniel Lüftner
Simulation of angle-resolved photoemission spectra by approximating the final state by a plane wave: from graphene to polycyclic aromatic hydrocarbon molecules
J. Elec. Spectr. Rel. Phen. **200**, 193-208 (2015)
http://dx.doi.org/10.1016/j.elspec.2015.06.003 (Hybrid OA)

[2] Hannes Offenbacher, Daniel Lüftner, Thomas Ules, Eva Maria Reinisch, Georg Koller, Peter Puschnig, and Michael G. Ramsey
Orbital tomography: molecular band maps, momentum maps and the imaging of real space orbitals of adsorbed molecules
J. Elec. Spectr. Rel. Phen. **200A**, 92-101 (2015)
http://dx.doi.org/10.1016/j.elspec.2015.04.023 (Hybrid OA)

[3] S. Weiß, D. Lüftner, T. Ules, E. M. Reinisch, H. Kaser, A. Gottwald, M. Richter, S. Soubatch, G. Koller, M. G. Ramsey, F. S. Tautz, and P. Puschnig
Exploring three-dimensional orbital imaging with energy dependent photoemission tomography
***Nature Communications* 6, 8287 (2015)**
http://dx.doi.org/10.1038/ncomms9287 (Hybrid OA)

[4] E. M. Reinisch, P. Puschnig, T. Ules, M. G. Ramsey, G. Koller
Layer-resolved photoemission tomography: The p-sexiphenyl bilayer upon Cs doping
Phys. Rev. B **93**, 155438 (2016)
http://dx.doi.org/10.1103/PhysRevB.93.155438
http://physik.uni-graz.at/~pep/P27649-N20/pdf/Reinisch2016.pdf (Green OA)

[5] Dario Knebl, Anton Hoerl, Andreas Truegler, Johannes Kern, Joachim R. Krenn, Peter Puschnig, and Ulrich Hohenester
Gap plasmonics of silver nanocube dimers
Phys. Rev. **B** 93, 081405(R) (2016)
http://dx.doi.org/10.1103/PhysRevB.93.081405
http://physik.uni-graz.at/~pep/P27649-N20/pdf/Knebl2016.pdf (Green OA)

[6] T. Ules, D. Lüftner, E. M. Reinisch, G. Koller, P. Puschnig, and M. G. Ramsey
Continuous or discrete: Tuning the energy level alignment of organic layers with alkali dopants
Phys. Rev. B **94**, 205405 (2016).
http://dx.doi.org/10.1103/PhysRevB.94.205405
http://physik.uni-graz.at/~pep/P27649-N20/pdf/Ules2016.pdf (Green OA)

[7] J. Gall, P. Zeppenfeld, L. Sun, L. Zhang, Y. Luo, Z. Dong, C. Hu, P. Puschnig
Spectroscopic STM studies of single pentacene molecules on Cu(110)_c(6x2)O
Phys. Rev. B **94**, 195441 (2016).
http://dx.doi.org/10.1103/PhysRevB.94.205144
http://physik.uni-graz.at/~pep/P27649-N20/pdf/Gall2016.pdf (Green OA)

[8] K. Schönauer, S. Weiss, V. Feyer, D. Lüftner, B. Stadtmueller, D. Schwarz, T. Sueyoshi, C. Kumpf, P. Puschnig, M. G. Ramsey, F. S. Tautz, S. Soubatch
Charge transfer and symmetry reduction at the CuPc/Ag(110) interface studied by photoemission tomography
Phys. Rev. B **94**, 205144 (2016).
http://dx.doi.org/10.1103/PhysRevB.94.205144
http://physik.uni-graz.at/~pep/P27649-N20/pdf/Schonauer2016.pdf (Green OA)

[9] A. Matkovic, J. Genser, D. Lüftner, M. K. R. Gajic, P. Puschnig, and C. Teichert
Epitaxy of highly ordered organic semiconductor crystallite networks supported by hexagonal boron nitride
Scientific Reports **6**, 38519 (2016).
http://dx.doi.org/10.1038/srep38519 (Hybrid OA)

[10] P. Puschnig, A. D. Boese, M. Willenbockel, M. Meyer, D. Lüftner, E. M. Reinisch, T. Ules, G. Koller, S. Soubatch, M. G. Ramsey, F. S. Tautz
On the energy ordering of molecular orbitals
***J. Phys. Chem. Lett.* 8, 208-213 (2017).**
http://dx.doi.org/10.1021/acs.jpclett.6b02517 (Hybrid OA)

[11] Christian Udhardt, Felix Otto, Christian Kern, Daniel Lüftner, Tobias Huempfner, Tino Kirchhuebel, Falko Sojka, Matthias Meissner, Bernd Schröter, Roman Forker, Peter Puschnig, Torsten Fritz
Influence of Film and Substrate Structure on Photoelectron Momentum Maps of Coronene Thin Films on Ag(111)
J. Phys. Chem. C **121**, 12285-12293 (2017).
http://dx.doi.org/10.1021/acs.jpcc.7b03500 (Hybrid OA)

[12] Hollerer, Michael and Lüftner, Daniel and Hurdax, Philipp and Ules, Thomas and Soubatch, Serguei and Tautz, Frank Stefan and Koller, Georg and Puschnig, Peter and Sterrer, Martin and Ramsey, Michael G.
Charge Transfer and Orbital Level Alignment at Inorganic/Organic Interfaces: The Role of Dielectric Interlayers
ACS Nano **11**, 6252-6260 (2017).
http://dx.doi.org/10.1021/acsnano.7b02449 (Hybrid OA)

[13] Giovanni Zamborlini, Daniel Lüftner, Zhijing Feng, Bernd Kollmann, Peter Puschnig, Carlo Dri, Mirko Panighel, Giovanni Di Santo, Andrea Goldoni, Giovanni Comelli, Matteo Jugovac, Vitaliy Feyer, and Claus Michael Schneider
Unexpected multi-orbital charge transfer at highly oriented organic/metal interfaces
Nature Communications **8**, 335 (2017).
http://dx.doi.org/10.1038/s41467-017-00402-0 (Hybrid OA)

[14] Daniel Lüftner, Simon Weiß, Philipp Hurdax, Xiaosheng Yang, Vitaly Feyer, Alexander Gottwald, Georg Koller, Serguei Soubatch, Peter Puschnig, Michael G. Ramsey, and F. Stefan Tautz
Understanding the photoemission distribution of strongly interacting two-dimensional overlayers
***Phys. Rev. B* 96, 125402 (2017).**
http://dx.doi.org/10.1103/PhysRevB.96.125402
http://physik.uni-graz.at/~pep/P27649-N20/pdf/Lueftner2017.pdf (Green OA)

[15] M. Graus, C. Metzger, M. Grimm, V. Feyer, P. Puschnig, A. Schöll, and F. Reinert
Degeneracy Lifting of Adsorbate Orbitals Imaged by High-Resolution Momentum Microscopy

Journal of the Physical Society of Japan **87**, 061009 (2018)
http://dx.doi.org/10.7566/JPSJ.87.061009 (Hybrid OA)

[16] Bernd Kollmann, Zhongrui Chen, Daniel Lüftner, Olivier Siri, and Peter Puschnig
Synthesis and combined experimental and theoretical characterization of dihydro-tetraaza-acenes
J. Phys. Chem. C **122**, 6475-6482 (2018).
http://dx.doi.org/10.1021/acs.jpcc.8b00985 (Hybrid OA)

[17] Yang, X.; Krieger, S. W. I.; Heepenstrick, T.; Hollerer, M.; Hurdax, P.; Lüftner, D.; Puschnig, P.; Koller, G.; Ramsey, M. G.; Sokolowski, M.; Tautz, F. S. & Soubatch, S.
On the decoupling of molecules at metal surfaces
Chem. Commun. **54**, 9039-9042 (2018).
http://dx.doi.org/10.1039/C8CC03334J (Green OA)

[18] Zamborlini, G.; Jugovac, M.; Floreano, L.; Verdini, A.; Cossaro, A.; Puschnig, P.; Lüftner, D.; Feyer, V. & Schneider, C. M
On-surface nickel porphyrin mimics reactive center of enzyme cofactor
Chem. Commun. **54**, 13423-13426 (2018).
http://dx.doi.org/10.1039/C8CC06739B (Green OA)

[19] Egger, L.; Kollmann, B.; Hurdax, P.; Lüftner, D.; Yang, X.; Weiß, S.; Gottwald, A.; Richter, M.; Koller, G.; Soubatch, S.; Tautz, F. S.; Puschnig, P. & Ramsey, M. G.
Can photoemission tomography be useful for small, strongly-interacting adsorbate systems?
New J. Phys. **21**, 043003 (2019).
http://dx.doi.org/10.1088/1367-2630/ab0781 (Hybrid OA)

1.2 Non peer-reviewed publications / already published (journals, monographs, anthologies, contributions to anthologies, research reports, working papers / preprints, proceedings, research data, etc.)

[B1] G. Koller, P. Puschnig, A. Gottwald, and F. S. Tautz
Elektronenorbitale in 3D - Photoelektronen-tomographische Bilder von Molekülorbitalen
Physik in unserer Zeit **47**, 192-198 (2016)
http://dx.doi.org/10.1002/piuz.201601442
http://physik.uni-graz.at/~pep/P27649-N20/pdf/Koller2016.pdf (Green OA)

[B2] Peter Puschnig and Michael G. Ramsey
Photoemission Tomography: Valence Band Photoemission as a Quantitative Method for Investigating Molecular Films
in: *Reference Module in Chemistry, Molecular Sciences and Chemical Engineering* 380-391 (2017).
http://dx.doi.org/10.1016/B978-0-12-409547-2.13782-5
http://physik.uni-graz.at/~pep/P27649-N20/pdf/Puschnig2017.pdf (Green OA)

1.3 Planned publications

Author(s)	Xiaosheng Yang , Larissa Egger, Philipp Hurdax, Hendrik Kaser, Daniel Lüftner, Francois C. Bocquet, Georg Koller, Alexander Gottwald, Petra Tegeder, Mathias Richter , Michael G. Ramsey , Peter Puschnig , Serguei Soubatch, F. Stefan Tautz		
Title	Identifying surface reaction intermediates with photoemission tomography		
Sources	submitted to Nature Communications		
URL (if applicable)			
Peer Review	yes ☒	no ☐	
Status	in press/accepted ☐	submitted ☒	in preparation ☐

Author(s)	Aleksandar Matković, Jakob Genser, Markus Kratzer, Daniel Lüftner, Zhongrui Chen , Olivier Siri, Peter Puschnig, Conrad Becker, and Christian Teichert		
Title	Light-assisted charge propagation in networks of organic semiconductor crystallite on hexagonal boron nitride		
Sources			
URL (if applicable)			
Peer Review	yes ☒	no ☐	
Status	in press/accepted ☐	submitted ☒	in preparation ☐

Author(s)	Xiaosheng Yang, Larissa Egger, Jana Fuchsberger, Martin Unzog, Daniel Lüftner, Felix Hajek, Philipp Hurdax, Matteo Jugovac, Giovanni Zamborlini, Vitaliy Feyer, Georg Koller, Michael G. Ramsey, Peter Puschnig, F. Stefan Tautz, and Serguei Soubatch		
Title	Electronic structure of tetracene on Ag(110) and Cu(110) studied by molecular orbital imaging		
Sources			
URL (if applicable)			
Peer Review	yes ☒	no ☐	
Status	in press/accepted ☐	submitted ☐	in preparation ☒

Author(s)	C. Metzger, M.Graus, M. Grimm, G. Zamborlini, V. Feyer, M. Schwendt, D. Lüftner, P. Puschnig, A. Schöll, and F. Reinert		
Title	Photoemission from fullerenes: A combined experimental and theoretical study on the example of the C60/Ag(110) interface		
Sources			
URL (if applicable)			
Peer Review	yes ☒	no ☐	
Status	in press/accepted ☐	submitted ☐	in preparation ☒

Author(s)	Norman Haag, Daniel Lüftner, Johannes Seidel, Peter Puschnig, Mirko Cinchetti, Benjamin Stadtmüller, Martin Aeschlimann		
Title	Exploring Photoemission Tomography of 3D Molecules in an Organic Crystal		
Sources			
URL (if applicable)			
Peer Review	yes ☒	no ☐	
Status	in press/accepted ☐	submitted ☐	in preparation ☒

Author(s)	Philipp Hurdax, Michael Hollerer, Martin Sterrer, Peter Puschnig, Daniel Lüftner, Larissa Egger and Michael G. Ramsey		
Title	Controlling the charge transfer across dielectric interlayers		
Sources			
URL (if applicable)			
Peer Review	yes ☒	no ☐	
Status	in press/accepted ☐	submitted ☐	in preparation ☒

Author(s)	Bernd Kollmann, Leeor Kronik, Peter Puschnig		
Title	Gas phase and solid state optical properties of indigo from an optimally-tuned range separated hybrid		
Sources			
URL (if applicable)			
Peer Review	yes ☒	no ☐	
Status	in press/accepted ☐	submitted ☐	in preparation ☒

2. Most important academic awards

(Specific academic awards, honours, prizes, medals or other merits)

Name of award	**n=national / i=international**

3. Information on results relevant to commercial applications

- Type of commercial application:
    1. Patent
    2. Licensing
    3. Copyrights (e.g. for software; no publications)
    4. Others

Type of commercial application		
Subject / title of the invention / discovery		
Short description of the invention / discovery		
Year		
Status	granted ☐	pending ☐
Application reference (or patent number)		

4. Publications for the general public and other publications

(Absolute figures, separate reporting of national / international publications)

- Type of dissemination activities:
    1. Self-authored publications on the World Wide Web
    2. Editorial contributions in the media (print, radio, TV, www, etc.)
    3. (Participatory) contributions within science communication
    4. Popular science contributions (books, lectures, exhibitions, films, etc.)

	national	**International**
Self-authored publications on the www	1	1
Editorial contributions in the media	1	1
(Participatory) contributions within science communication		
Popular science contributions	1	

5. Development of collaborations

Indication of the most important collaborations (no more than 5) that took place (i.e. were initiated or continued) in the course of the project. Please provide the name of the collaboration partner (name, title, institution) and a few words about the scientific content. Please **categorise** each collaboration arrangement as follows:

N				Nationality of collaboration partner (please use the ISO-3-letter country code)
	G			Gender **F (**female) **M** (male)
		E		Extent **E1** **low** (e.g. no joint publications, but mention in acknowledgements or similar); **E2** **medium** (collaboration e.g. with occasional joint publications, exchange of materials or similar, but no longer-term exchange of personnel); **E3** **high** (extensive collaboration with mutual hosting of group members for research stays, regular joint publications, etc.)
			D	Discipline **W** **within the discipline** (within the same scientific field) **I** **interdisciplinary** (involving two or more disciplines) **T** **transdisciplinary** (collaborations outside the sciences)

N	**G**	**E**	**D**	**Name**	**Institution**
AUT	M	E3	I	Prof. M. G. Ramsey	University Graz
DEU	M	E3	I	Prof. F. S. Tautz	Forschungszentrum Jülich
DEU	M	E2	I	Prof. C. M. Schneider	Forschungszentrum Jülich
ISR	M	E2	W	Prof. L. Kronik	Weizmann Institute of Science
AUT	M	E2	W	Prof. A. D. Boese	University Graz

Note: General scientific contact and occasional meetings should not be considered collaborations for the purposes of this report.

6. Development of human resources in the course of the project

(Absolute figures with an indication of status (in progress / completed)

Note: It is not possible to assign a *venia* thesis / work (*Habilitation*) to a single project; here it is necessary to mention those *venia* theses for which the project was important. A similar caveat applies to Ph.D. and diploma theses: The FWF does not support thesis work, but instead funds the scientific work that forms the basis for such theses.

	In progress	**Completed**	**Gender**	
			f	**m**
Full professorship				
Venia thesis (*Habilitation*) / Equivalent senior scientist qualification				
Postdoc		1		1
Ph.D. theses	1	2	1	2
Master's theses	2	2	1	3
Diploma theses				
Bachelor's theses	2			2

7. Applications for follow-up projects

(Please indicate the status of each project and the funding organisation)

7.1 Applications for follow-up projects (FWF projects)

Please indicate the project type (e.g. stand-alone project, SFB, DK, etc.)

Project number (if applicable)	I 3731		
Project type	D.A.CH project		
Title / subject	Exploring the foundations of photoemission tomography		
Status	granted ☒	pending ☐	in preparation ☐
Application reference (if a patent is applied)			

Project number (if applicable)	I 4145 (PI = Georg Koller, 1 PhD position for Puschnig-group)		
Project type	Internationale Projekte		
Title / subject	Photoemission Tomography of Excited Molecular States		
Status	granted ☒	pending ☐	in preparation ☐
Application reference (if a patent is applied)			

7.2 Applications for follow-up projects (Other national projects)

(e.g. FFG, CD Laboratory, K-plus centres, funding from the Austrian central bank [OeNB], Austrian federal government, provincial agencies, provincial government or similar sources)

Funding agency	Please choose an item: Wählen Sie ein Element aus.		
Other national funding agencies			
Project number (if applicable)			
Project type			
Title / subject			
Status	granted ☐	pending ☐	in preparation ☐
Total costs (granted)			

7.3 Applications for follow-up projects (international projects) (e.g. EU, ERC or other international funding agencies)

Country			
Funding agency	Please choose an item: Wählen Sie ein Element aus.		
Project number (if applicable)			
Project type			
Title / subject			
Status	granted ☐	pending ☐	in preparation ☐
Total costs (granted)			

IV. Cooperation with the FWF

Please rate the following aspects with regard to your interaction with the FWF. Please provide any **additional comments (explanations)** on the supplementary sheet with a reference to the corresponding question/aspect.

Scale:
-2 highly unsatisfactory
-1 unsatisfactory
0 appropriate
+1 satisfactory
+2 highly satisfactory
X not used

Rules
(i.e. guidelines for: funding programme, application, use of resources, reports)

		Rating
Application guidelines	Length	**+2**
	Clarity	**+2**
	Intelligibility	**+2**

Procedures (submission, review, decision)

	Advising	**+1**
	Duration of procedure	**0**
	Transparency	**+1**

Project support

Advising	Availability	**+1**
	Level of detail	**+1**
	Intelligibility	**+1**

Financial transactions (credit transfers, equipment purchases, personnel management)	

Reporting / review / exploitation

	Effort	**+1**
	Transparency	**+1**
	Support in PR work / exploitation	**X**

Comments on cooperation/interaction with the FWF: