STAND-ALONE PROJECT

FINAL REPORT

P23190-N16   **Project number**

Project title[1]   **Understanding photoemission of organic molecular films**

Theoretische Beschreibung der Photoemission von organischen Molekülfilmen

Project leader   **Assoz.-Prof. Dr. Peter Puschnig**

Project website[2]   **http://physik.uni-graz.at/~pep/P23190-N16/index.html**

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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

In diesem Projekt wurde der Photoemissionsprozess von dünnen, organischen Molekülfilmen, die auf Metalloberflächen adsorbiert sind, mithilfe eines quantenmechanischen *ab-initio* Verfahrens theoretisch untersucht. Es konnte gezeigt werden, dass die Winkelabhängigkeit des Photostroms von solchen Molekülfilmen – im Gegensatz zur allgemeinen Annahme – durch einen sehr einfachen Ansatz für den Endzustand der Photoemission, nämlich einen freien Elektronenzustand, beschrieben werden kann. Diese Methode ermöglichte eine einfache und intuitive Interpretation der Messdaten mit Hilfe einer Fourier-Transformation der Wellenfunktion des Anfangszustands der Photoemission. Dieser Zusammenhang zieht eine Reihe von faszinierenden Anwendungen nach sich und wurde von uns als Methode der „Orbitaltomographie" bezeichnet. Beispielsweise ist es möglich die Elektronenverteilung einzelner Molekülorbitale im Realraum aus den Messdaten zu bestimmen, und das in entweder in zwei oder sogar in drei Raumdimensionen. Wir konnten auch zeigen, dass sogar die Phaseninformation der Wellenfunktion aus den Photoemissionsmessungen rekonstruiert werden kann. Nicht zuletzt liefert die Orbitaltomographie auch sehr detaillierte Aussagen über die Energieposition und den Charakter von einzelnen Molekülzuständen und deren Wechselwirkung mit Metalloberflächen, was wiederum wichtige Impulse für die weitere Entwicklung von ab-initio Methoden zur elektronischen Strukturberechnung bringt.

Diese grundlegenden Untersuchungen der Grenzflächen zwischen organischen Molekülen und Metalloberflächen können in Zukunft dazu beitragen, die Eigenschaften von organischen Halbleiterbauelementen weiter zu verbessern. Ultradünne Schichten aus organischen Molekülen sind die Basis einer neuartigen Halbleitertechnologie, in der biegsame Displays oder kostengünstige Photovoltaik-Zellen mögliche Anwendungen darstellen. Für einen erfolgreichen Einsatz in organischen Halbleiterbauelementen ist jedoch ein fundamentales Verständnis der elektrischen und optischen Eigenschaften an der Molekül / Metall Grenzfläche erforderlich. Insbesondere werden diese Eigenschaften ja durch die fundamentalen Wechselwirkungen der Molekülorbitale mit den Elektronenzuständen an der Metalloberfläche bestimmt. Und daher sind Methoden, die die räumliche Lage sowie die energetische Position der Grenzflächenzustände zugänglich machen, wie eben die Verfahren, die in diesem Projekt entwickelt und angewendet wurden, wichtige Hilfsmittel, um die Effizienz von organischen Halbleitern in Zukunft weiter steigern zu können.

2.   Summary for public relations work

This project has theoretically investigated the photoemission process from organic molecular films by employing a quantum-mechanical first-principles approach. It could be shown that – opposite to the general belief – the angular dependence of the photoemission current from oriented molecular films can be well understood by assuming a plane wave as the final state of the photoemission process. The method enabled a simple and intuitive interpretation of the measurement data in terms of the Fourier transform of the initial state orbital and has opened a number of fascinating perspectives. The reconstruction of the real space electron distribution of individual molecular orbitals could be demonstrated in two and three spatial dimensions, a procedure to recover the phase information of the quantum mechanical wave function from experimental data was developed, and stringent benchmarks for the further development of ab-initio electronic structure theories could be derived.

These fundamental investigations of the interface between organic molecules and metallic surfaces are envisioned to facilitate the tailoring of organic semiconductor interfaces with desired properties in future. Ultra-thin films made of organic molecules form the basis of novel semiconductor technologies. Because organic molecules are extremely flexible, they can be used in a whole new range of applications, making it equally possible to create pliable screens and cost-effective photo-voltaic cells. A successful application of organic semiconductors in such devices, however, asks for a better understanding of the fundamental interactions between the organic material and the inorganic carrier substances. These interactions are largely determined by the molecule's frontier orbitals, i.e., the highest occupied and the lowest unoccupied molecular orbital. Methods to determine their spatial distribution, such as the ones developed in this project, will allow for to better understanding of how organic semiconductor components work and thus help to improve their efficiency.

II. Brief project report

1. Report on research work

1.1 Information on the development of the research project

Overall scientific concept and goals. The project "Understanding photoemission from organic molecular films" that has been formulated in July 2010 and been started in May 2011 deals with the ab-initio simulation of the angle-resolved photoemission (PE) from organic molecular films based on the one-step model of photoemission. In the proposal, the research goals have been grouped into five topics. For convenience, these are briefly summarized here.

(A) Substrate effects. In previous applications of the one-step model to compute the PE intensity from molecular layers, the initial state orbital has been taken from DFT calculations for isolated molecules. Thus, effects of the substrate and possible intermolecular interactions have been disregarded. However, for rather strongly bound organic molecular monolayers adsorbed on metallic surfaces, the photoemission cross section will certainly be modified compared to a decoupled organic layers. Within this proposal, it was thus planned to extend the evaluation of the PE from isolated molecule initial states to Bloch states produced from ab-initio electronic structure calculations of the full molecule / substrate system.

(B) Beyond the plane wave final state. By assuming a plane wave for the final state, the evaluation greatly simplifies. We could prove the usefulness of this simple relation in previous publications. In this project, it was planned to investigate how deviations from these requirements affect validity of the PW final state assumption.

(C) Orbital energies. It was also planned go beyond standard LDA and GGA functionals and apply hybrid exchange correlation functionals which were found to mitigate effects of the self-interaction error significantly via the inclusion of a fraction of Fock exchange. It was intended to utilize the non-empirical PBE0 hybrid functional which was shown to provide computed photoemission spectra of organic molecules in excellent agreement with experimental data. It was also planned to implement approximate schemes to estimate self-interaction corrected eigenvalues which are based purely on LDA quantities. Alternatively, also computations of quasi-particle energies by solving Hedin's quasi-particle equations by using the GW approximation for the self-energy operator were envisioned.

(D) 3D orbital imaging. Within the PW final state approximation, the one-step model connects the angle-dependent photocurrent for a given kinetic energy with the Fourier transform of the electron distribution at the initial state energy for a constant absolute value of the wave vector. If the photocurrent is measured for varying final state kinetic energies, i.e., by increasing the photon energy and keeping the initial state energy constant, different hemispherical sections of the molecular orbital in reciprocal space are probed. Based on experimental data sets with varying photon energies, it was planned to investigate the possibility to obtain the three-dimensional electron distribution in individual molecular orbitals.

(E) Recovery of phase information. The measured ARPES intensity is proportional to the absolute value of the molecular orbital in momentum space. The phase information, however, is experimentally not accessible. Within this project, it was planned to develop a general procedure which to recover the phase information.

In the course of the project (May 2011 – May 2014), almost all research questions summarized above could be tackled and led to a number of publications (see part III, 1.1). Substrate effects (A) are discussed in [6, 9, 15, 18], the question of accurate orbital energies (C) are treated in [1, 3, 7, 12, 13, 14, 17, 20], orbital imaging in 3D (D) was just recently

studied in [21], and a procedure for recovering the phase information (E) was developed and applied in [11, 19]. Since experimental indications for effects beyond the plane wave final state turned out to be weaker than expected, this research question (B) has been postponed and is in fact now one of the central topics in the follow-up project P27649-N20 (Quantifying photoemission from organic molecular films). Rather has the plane wave final state approximation turned out to be extremely useful in interpreting experimental data and has led to the development of a technique which we termed orbital tomography, see [1, 4, 5, 7, 12, 13, 14, 15].

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

Development of new methods. We have developed a technique which we termed "Orbital Tomography" which is based on a comparison between experimental ARPES data recorded over a wide kx-ky-range (momentum map) with simulations based on the plane wave final state. It allows one to deconvolute spectra into individual orbital contributions and thus provides an orbital-by-orbital characterization of large adsorbate systems allowing one to directly estimate the effects of bonding on individual orbitals. Moreover, *orbital tomography*, yields most stringent tests for ab initio electronic structure theory. This method was published in Physical Review B in 12/2011 [1] (endowed with an Editor's Suggestion) and has already been cited 47 times. Thereby, we are able to disentangle the valence band spectrum of molecular films into contributions from various molecular orbitals. Subsequently, the orbital tomography approach has been applied to a number of similar organic/metal interfaces. These applications include nanoscale-graphene molecules [4,20], the identification of doping states of Cs-doped sexiphenyl [12], and the determination of the azimuthal alignment of Cu-phthalocyanine [14] and tetra-phenyl-porphyrines [8]. Orbital tomography was also generalized to highly-symmetric surfaces with multiple domain orientations of molecular islands [5]. This allowed us to investigate the energy splittings arising from intermolecular interactions [7], or to analyze the nature of the frontier molecular orbitals in organic heteromolecular hybrid interfaces [13]. Also, other groups have adopted the orbital tomography approach in order to tackle similar problems.

Breaking of new scientific / scholarly ground. The basis for a quantum-mechanical description of matter is electron wave functions. For atoms and molecules, their spatial distributions and phases are known as orbitals. Although orbitals are very powerful concepts, experimentally only the electron densities and -energy levels are directly observable. Regardless whether orbitals are observed in real space with scanning probe experiments, or in reciprocal space by photoemission, the phase information of the orbital is lost. In [11], we show that the experimental momentum maps of angle-resolved photoemission from molecular orbitals can be transformed to real-space orbitals via an iterative procedure which also retrieves the lost phase information. This is demonstrated with images obtained of a number of orbitals of the molecules pentacene ($C_{22}H_{14}$) and perylene-3,4,9,10-tetracarboxylic dianhydride ($C_{24}H_8O_6$), adsorbed on silver, which are in excellent agreement with ab initio calculations. The procedure requires no a priori knowledge of the orbitals and is shown to be simple and robust. Recently, this iterative procedure has also been applied to recover a number of sexiphenyl ($C_{36}H_{26}$) orbitals from ARPES data [19].

Contribution to the advancement of the field. The project also contributed to the question on how well orbital energies from density functional theory approximate electron removal energies as measured by photoemission experiments. Self-interaction errors present in local (LDA) or semi-local functionals (GGA) may lead to wrong orbital energies sometimes even wrong orbital ordering. We have performed several hybrid functional calculations, both, for isolated molecules as well as for molecules adsorbed on metallic surfaces which have been shown to mitigate these problems. In [1], we have applied the range-separated hybrid functional HSE to PTCDA in the gas phase, and also applied a simplified SIE correction-scheme. It is shown that, compared to experiment, this not only improves the energetic position of the di-anhydride-related sigma-orbitals, but also provides a better description of the lower lying pi-states. For Cu-phthalocyanine/Au(110) [14], we were able to compute the electronic structure of the adsorbed system within GGA and the hybrid functional HSE. We have also studied pentacene monolayers on the Ag(110) and Cu(110) surfaces, both, within GGA and within the hybrid functional HSE [15]. For both surfaces we find that HSE improves the agreement with experiment in terms of the energy position of several molecular states including the LUMO, HOMO and HOMO-1. For a model system, poly-para-phenylene adsorbed on graphene, the band gap narrowing of the polymer upon adsorption on graphene due to polarization effects could be demonstrated by performing GW-calculations [3].

In collaboration with Prof. Kronik, we have employed an optimally-tuning approach to determine all parameters in a general range-separated hybrid functional (OT-RSH) by physical constraints. We partition the Coulomb interaction into a short-range part and a long-range part and enforce the correct $1/r$ asymptotic behavior at long range for the isolated molecule. Moreover, we tune the range-separation parameter, such that the ionization-potential (IP) theorem is obeyed. We have applied this approach to the organic molecule quinacridone in the gas phase and in the bulk phase [17]. We found that all OT-RSH results, almost independent of the amount of Hartee-Fock exchange (alpha), provide excellent values for the IP and the HOMO-LUMO gap, while alpha controls the relative position of the sigma and pi orbitals [17]. In collaboration with Prof. Kümmel [16], the foundations of the molecular orbital interpretation in performing ARPES experiments have been investigated.

Most important hypotheses / research questions. Most of the questions raised in the proposal from July 2010 could be already tackled, some problems were left open, and a number of new issues arose in the course of the project. These are briefly summarized below and have led to the follow-up proposal entitled "Quantifying photoemission of organic molecular films" funded by the FWF under project number P27649-N20.

The orbital tomography approach developed within the current P23190-N16 project has certainly contributed to shed light on the physics of angle-resolved photoemission from organic molecular films. However, there are a number of problems which require a more refined theoretical treatment. This will allow for a quantitatively precise analysis of experimental data. The theoretical refinements regard, both, the description of the initial and final states, as well as the coupling of the electron system to the photon field. First, it will be necessary to compute accurate initial state energies. This means that one has to go beyond GGA and apply hybrid functional and/or leave DFT and perform quasi-particle calculations within the GW approximation. While such research activities have already proven fruitful in the current project, G0W0 results based on an appropriate starting point for organic/metal interfaces would be highly desirable but have proven prohibitive to-date. Second, it ought to be tested how sensitive ARPES simulations are with respect to approximations for the initial

state wave function. So far, only GGA wave functions have been used, but it would be highly interesting to explore, for instance, how the correct asymptotic tail of the wave function obtained from a hybrid DFT calculation with a proper asymptotic long-range behavior or from self-consistent GW calculations would affect the ARPES intensity. Third, even though the plane wave approximation for the final state has proven successful for many systems studied so far, it is clearly limited. In particular, it may be expected to show problems when attempting to account for the photon energy dependence of ARPES data, which is necessary in order to retrieve three-dimensional information of the orbital. As a last point, the role of the photon polarization on the observed ARPES intensity needs to be explored in more detail. In particular, it has been recently suggested that the circular dichroism in the angular distribution (CDAD) of the photocurrent can be exploited to determine the phases of the initial state wave function from experiment only. More theoretical work would be necessary to shed light on this fascinating idea.

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 started in May 2011 at the University of Leoben (Chair of Atomistic Modelling and Design of Materials), has moved the Unversity of Graz (Institute of Physics) in February 2012, and has ended in May 2015.

Use of personnel. Dr. Matus Milko was employed as a PostDoc from 06/2011 – 02/2013, and Dipl.-Ing. Lüftner as a PhD from 09/2011 – 04/2015 (Rigorosum in 05/2015). In addition Bernd Kollmann was employed as a PhD from 02/2015 – 05/2015, and Dr. Margareta Wagner as a short-term PostDoc from 08/2012 – 09/2012.

Major items of equipment purchased. A computer cluster with 56 compute-cores was bought in May/2011 which is currently still in use and has been very important for performing the computations achieved in this project.

Other significant deviations. The project duration was extended by 1 year with no additional costs.

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

Peter Puschnig: In the course of the project, the PI moved from Leoben University (Research Assistant position) to the University of Graz in February 2012 where he attained a tenured Assistant Professorship. Not least owing to publication originating from this project, in March 2014, the position was transformed into a permanent Associate Professor position.

Matus Milko: He was employed as a PostDoc from 06/2011 – 02/2013 after which he decided to leave academia and start a career in industrial research.

Daniel Lüftner: He conducted his PhD thesis which has been compiled in the form of a cumulative thesis owing to the large number and excellent quality of his publication work during the course of the project. He attained his Doctoral degree in May 2015, and is currently employed as a PostDoctoral Researcher until 09/2016 in the framework of the follow-up project.

Bernd Kollmann: He conducted his master thesis in a topic related to the project which qualified him as an excellent candidate for a PhD in the follow-up project.

Dario Knebl: He also conducted his master thesis in a topic related to the project which. This has qualified him to conduct a PhD thesis which is aiming at bridging the gap between the field of plasmonic nanoparticles and electronic structure theory of molecules interacting with

metallic nanoparticles (thesis supervised by Prof. Ulrich Hohenester, KFU Graz, co-supervised by the PI).

3. Effects of the project beyond the scientific field

On four occasions, project publications have been accompanied by press releases:

February 2013: Paper in Nature Communications "Substrate-mediated band-dispersion of adsorbate molecular states" [6] with the press release: "Kommunikation auf Umwegen" http://www.uni-wuerzburg.de/sonstiges/meldungen/single/artikel/kommunikat-2/

December 2013: Paper in the Proceedings of the National Academy of Sciences: "Imaging the wave functions of adsorbed molecules" [11]: "Vermessung von Molekülen" https://offeneslabor.uni-graz.at/de/neuigkeiten/detail/article/vermessung-von-molekuelen-4/

April 2014: Paper in Nature Communications: "Unexpected interplay of bonding height and energy level alignment at heteromolecular hybrid interfaces" [13]: "Wenn die Chemie stimmt" http://on.uni-graz.at/de/forschen/article/wenn-die-chemie-stimmt-3/

September 2015: Paper in Nature Communications: "Exploring three-dimensional orbital imaging with energy dependent photoemission tomography" [21]: "Grazer Physiker gewähren atomare Einblicke in 3D"
https://science.apa.at/rubrik/natur_und_technik/Grazer_Physiker_gewaehren_atomare_Einblicke_in_3D/SCI_20151005_SCI39391351425880628"

4. Other important aspects (examples)

Selected conference participations (a full list is available online: http://physik.uni-graz.at/~pep/P23190-N16/publications.html)

02/2012: Peter Puschnig, March meeting of the American Physical Society, Boston, USA February 27th - March 2nd 2012, "Orbital tomography: Deconvoluting photoemission spectra of organic molecules"

09/2013: Peter Puschnig, Joint Meeting of the Austrian and Swiss Physical Society (invited talk), University Linz, September 4th 2013. "Organic Semiconductors Explored With Ab-initio Electronic Structure Methods"

03/2014: Peter Puschnig, DPG meeting, TU Dresden, March 30th - April 4th, 2014.
"The Electronic Structure of Quinacridone: Optimally-Tuned Range-Separated Hybrid Functional versus GW Results"

03/2015: Peter Puschnig, 79. Jahrestagung der DPG und DPG-Frühjahrstagung, Berlin, 15. - 20. März 2015. "Orbital tomography: beyond the plane wave final state approximation"

Prizes/awards
11/2014 Daniel Lüftner is awarded the Nano-Prize of the Erwin Schroedinger Society for his work on the reconstruction of molecular orbitals from photoemission data. Press release: https://www.uni-graz.at/de/mitarbeiten/mitarbeiterinnen/karriere-ehrungen/ehrungen/detail/article/der-nano-meister-1/
Print media coverage:
https://www.kleinezeitung.at/s/steiermark/steirerdestages/4613151/PREISTRAeGER_Wellenfunktion-uberlistet

III. Attachments

1. Scholarly / scientific publications

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

[1] P. Puschnig, E.- M. Reinisch, T. Ules, G. Kollerm S. Soubatch, M. Ostler, L. Romaner, F. S. Tautz, C. Ambrosch-Draxl, M. G. Ramsey, Orbital tomography: Deconvoluting photoemission spectra of organic molecules, Phys. Rev. B 84, 235427 (2011), http://dx.doi.org/10.1103/PhysRevB.84.235427 (Hybrid OA:).

[2] J. Henzl, P. Puschnig, C. Ambrosch-Draxl, A. Schaate, B. Ufer, P. Behrens, K. Morgenstern, Photoisomerization for a molecular switch in contact with a surface, Phys. Rev. B 85, 035410 (2012), http://dx.doi.org/10.1103/PhysRevB.85.035410 (Green OA: http://unipub.uni-graz.at/obvugroa/content/titleinfo/762956).

[3] P. Puschnig, P. Amiri, C. Draxl, Band renormalization of a polymer physisorbed on graphene investigated by many-body perturbation theory, Phys. Rev. B 86, 085107 (2012), http://dx.doi.org/10.1103/PhysRevB.86.085107, (Green OA, http://arxiv.org/abs/1204.5289)

[4] M. Wießner, N.S. Rodriguez-Lastra, J. Ziroff, F. Forster, P. Puschnig, L. Dössel, K. Müllen, A. Schöll, and F. Reinert, The electronic structure of nanoscale graphene: molecular versus quantum-dot viewpoint, New Journal of Physics 14, 113008 (2012), http://dx.doi.org/10.1088/1367-2630/14/11/113008 (Hybrid OA)

[5] B. Stadtmüller, M. Willenbockel, E.M. Reinisch, T. Ules, M. Ostler, F. Bocquet, S. Soubatch, P. Puschnig, G. Koller, M. G. Ramsey, F. S. Tautz, and C. Kumpf, Orbital tomography for highly symmetric adsorbate systems, European Physics Letters 100, 26008 (2012), http://dx.doi.org/10.1209/0295-5075/100/26008 (Green OA: http://unipub.uni-graz.at/obvugroa/content/titleinfo/762988)

[6] M. Wießner, J. Ziroff, F. Forster, M. Arita, K. Shimada, P. Puschnig, A. Schöll, and F. Reinert, Substrate-mediated band-dispersion of adsorbate molecular states, Nature Communications 4, 1514 (2013), http://dx.doi.org/10.1038/ncomms2522 (Green OA, http://physik.uni-graz.at/~pep/Publications/Wiessner2012b.pdf, http://unipub.uni-graz.at/obvugroa/content/titleinfo/762965)

[7] M. Willenbockel, B. Stadtmüller, K. Schönauer, F. Bocquet, D. Lüftner, E.M. Reinisch, T. Ules, G. Koller, C. Kumpf, S. Soubatch, P. Puschnig, M. G. Ramsey, F. S. Tautz, Energy offsets within a molecular monolayer: The influence of the molecular environment, New Journal of Physics 15, 033017 (2013). http://dx.doi.org/10.1088/1367-2630/15/3/033017 (Hybrid OA)

[8] Margareta Wagner, Peter Puschnig, Stephen Berkebile, Falko P. Netzer, and Michael G. Ramsey, Alternating chirality in the monolayer H2TPP on Cu(110)-(2x1)O, Phys. Chem. Chem. Phys. 15, 4691-4698 (2013), http://dx.doi.org/10.1039/C3CP44239J (Hybrid OA).

[9] M. Wießner and J. Kuebert and V. Feyer and P. Puschnig and A. Schöll and F. Reinert, Lateral band formation and hybridization in molecular monolayers: NTCDA on Ag(110) and Cu(100), Phys. Rev. B 88, 075437 (2013), http://dx.doi.org/10.1103/PhysRevB.88.075437 (Green OA: http://unipub.uni-graz.at/obvugroa/content/titleinfo/762947)

[10] M. Monazam, K. Hingerl, and P. Puschnig, Quasiparticle band structure and optical properties of the alpha-12 Si-Ge superstructure from first principles, Phys. Rev. B 88, 075314 (2013), http://dx.doi.org/10.1103/PhysRevB.88.075314 (Green OA: http://arxiv.org/abs/1508.04550).

[11]   D. Lüftner, T. Ules, E.M. Reinisch, G. Koller, S. Soubatch, F. S. Tautz, M. G. Ramsey, and P. Puschnig, Imaging the wave functions of adsorbed molecules, Proc. Natl. Aca. Sci. (PNAS) 111, 605-610 (2014), http://dx.doi.org/10.1073/pnas.1315716110 (Hybrid OA)

[12]   E. M. Reinisch, T. Ules, P. Puschnig, S. Berkebile, M. Ostler, T. Seyller, M. G. Ramsey and G. Koller, Development and character of gap states on alkali doping of molecular films, New Journal of Physics 16, 023011 (2014), http://dx.doi.org/10.1088/1367-2630/16/2/023011 (Hybrid OA)

[13]   B. Stadtmüller, D. Lüftner, M. Willenbockel, E. M. Reinisch, T. Sueyoshi, G. Koller, S. Soubatch, M. G. Ramsey, P. Puschnig, F. S. Tautz, and C. Kumpf, Unexpected interplay of bonding height and energy level alignment at heteromolecular hybrid interfaces, Nature Communications 5, 3685 (2014), http://dx.doi.org/10.1038/ncomms4685 (Green OA: http://physik.uni-graz.at/~pep/P23190-N16/pdf/Stadtmuller2013.pdf)

[14]   D. Lüftner, M. Matus Milko, S. Huppmann, M. Scholz, N. Ngyuen, M. Wiessner, A. Schöll, F. Reinert, and P. Puschnig, CuPc/Au(110): Determination of the azimuthal alignment by combination of a angle-resolved photoemission and density functional theory, Journal of Electron Spectroscopy and Related Phenomena 195, 293-300 (2014), http://dx.doi.org/10.1016/j.elspec.2014.06.002 (Hybrid OA).

[15]   Thomas Ules, Daniel Lüftner, Eva Maria Reinisch, Georg Koller, Peter Puschnig, and Michael G. Ramsey, Orbital Tomography of Hybridized and Dispersing Molecular Overlayers, Phys. Rev. B 90, 155430 (2014), http://dx.doi.org/10.1103/PhysRevB.90.155430 (Green OA: http://arxiv.org/abs/1508.04547).

[16]   M. Dauth, M. Wießner, V. Feyer, A. Schöll, P. Puschnig, F. Reinert, and S. Kümmel, Angle resolved photoemission from organic semiconductors: orbital imaging beyond the molecular orbital interpretation, New Journal of Physics 16, 103005 (2014), http://dx.doi.org/10.1088/1367-2630/16/10/103005 (Hybrid OA).

[17]   Daniel Lüftner, Sivan Refaely-Abramson, Michael Pachler, Roland Resel, Michael G. Ramsey, Leeor Kronik, and Peter Puschnig, Experimental and theoretical electronic structure of quinacridone, Phys. Rev. B 90, 075204 (2014), http://dx.doi.org/10.1103/PhysRevB.90.075204 (Green OA: http://arxiv.org/abs/1508.04545).

[18]   M. Willenbockel, D. Lüftner, P. Puschnig, C. Kumpf, S. Soubatch, M. G. Ramsey, and F. S. Tautz, The interplay between interface structure, energy level alignment and chemical bonding strength at organic-metal interfaces, Phys. Chem. Chem. Phys. 17, 1530-1548 (2015), http://dx.doi.org/10.1039/C4CP04595E (Green OA: http://physik.uni-graz.at/~pep/P23190-N16/pdf/Willenbockel2014.pdf).

[19]   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, invited paper: J. Elec. Spectr. Rel. Phen. 204A, 92-101 (2015), http://dx.doi.org/10.1016/j.elspec.2015.04.023 (Hybrid OA).

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

[21]   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://www.nature.com/ncomms/2015/151005/ncomms9287/full/ncomms9287.html
(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.)

[1]   Peter Puschnig, Georg Koller, Claudia Draxl and Michael G. Ramsey, "The Structure of Molecular Orbitals Investigated by Angle-Resolved Photoemission", Small Molecules on Surfaces - Fundamentals and Applications (Springer Series in Materials Science 173, 2013). http://dx.doi.org/10.1007/978-3-642-33848-9_1 (Green OA: http://physik.uni-graz.at/~pep/P23190-N16/pdf/Puschnig2012a.pdf)

1.3 Planned publications
(journals, monographs, anthologies, contributions to anthologies, proceedings, research data, etc.)

Author(s)	E. M. Reinisch, P. Puschnig, T. Ules, G. Koller, and M. G. Ramsey
Title	p-Sexiphenyl bilayer on Cu(110) upon Cs-doping – layer resolved photoemission tomography
Sources	
URL (if applicable)	
Peer Review	yes ☒ no ☐
Status	in press/accepted ☐ submitted ☐ in preparation ☒

Author(s)	D. Lüftner, P. Puschnig, M. G. Ramsey, and F. S. Tautz
Title	The Orbital Tomography Technique (to appear in: Springer book series)
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
Daniel Lüftner, "Nano-Prize" of the Erwin Schrödinger Society for Nanosciences, November 2014	N

3.   Information on results relevant to commercial applications

Not applicable.

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	2	-
Editorial contributions in the media	2	-
(Participatory) contributions within science communication	-	-
Popular science contributions	-	-

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	W	Prof. S. Kümmel	University Bayreuth

N	G	E	D	Name	Institution
AUT	M	E3	I	Prof. M. G. Ramsey	University Graz
DEU	M	E2	I	Prof. A. Schöll	University Würzburg
ISR	M	E2	W	Prof. L. Kronik	Weizmann Institute of Science
DEU	W	E2	W	Prof. C. Draxl	Humboldt University Berlin

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		2
Ph.D. theses	1	3	1	3
Master's theses		2		2
Diploma theses				
Bachelor's theses				

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)   **P27649-N20**
Project type   **Single project**
Title / subject   **Quantifying photoemission from organic molecular films**
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	+1
	Transparency	+1

Project support

Advising	Availability	+2
	Level of detail	+1
	Intelligibility	+2

Financial transactions (credit transfers, equipment purchases, personnel management)	+2

Reporting / review / exploitation

Effort	+2
	+1

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

Comments on cooperation/interaction with the FWF: