Christoph Wolf

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Group Leader *Theory of Quantum Systems at Surfaces* at Center for Quantum Nanoscience

Center for Quantum Nanoscience (QNS)
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Short Biography:

I joined QNS in fall of 2017 as a post-doc after obtaining my PhD from POSTECH University earlier that year. My work focuses on computational modeling of quantum coherent properties of localized electron spins on and near surfaces. Since September of 2020 I lead my own research group called *Theory of Quantum Systems at Surfaces* in QNS. Together with my team I focus on the development of predictive methods for the discovery, optimization, and control of quantum spin systems.

Research Interests and Qualifications:

- **Open quantum systems simulations**: simulation of quantum-coherent properties of closed and open quantum systems, focusing on achieving quantum-optimal control of surface spin systems
- **Non-equilibrium quantum transport**: non-equilibrium Green's functions (NEGF) method for electron spin resonance (ESR) in the scanning tunneling microscope (STM), development of time-dependent ESR code to study the current-induced decoherence of quantum spin impurities under bias
- **Ab initio and ab initio-based methods**: density functional theory (DFT) and multiplet calculation for correlated electron systems to find and optimize localized spin systems with favorable properties for quantum information application

Education:

2014 – 2017: PhD. In Materials Science and Engineering, POSTECH University, Pohang, South Korea

Thesis title: Excitons and Phonons in Lead-Halide Perovskites (Advisor: Jung Kyu Kim)

2012 – 2014: Master's degree in Engineering Physics, University of Technology Graz, Austria

Thesis title: Investigation of the switching mechanism in metal/organic/metal thin film devices (Advisor: Emil J.W. List-Kratochvil)

2008 – 2012: Bachelor's degree in Engineering Physics, Graz, Austria

Professional Appointments:

2020/09 – now:	Research Professor at EWHA Womans University and Group leader (PI) at the Center for Quantum Nanoscience
2017/10-2020/09:	Post-doc, Center for Quantum Nanoscience
	Supervisor: Andreas J. Heinrich
2017/06-2017/09:	Post-doc, Printed Nano-electronics lab (PNEL), Seoul National University
	Supervisor: Tae-Woo Lee

Research Stays:

2019/08-09:	Materials Physics Center (CFM), Donostia, Spain. (Collaborator: Nicolas Lorente)
2018/09-10:	Materials Physics Center (CFM), Donostia, Spain. (Collaborator: Nicolas Lorente)
2018/03-05:	Materials Physics Center (CFM), Donostia, Spain (Collaborator: Nicolas Lorente)

Teaching Experience:

2021 fall:	Quantum Computing, Co-instructor (graduate level)
2021 spring:	Solid State Physics, leading exercise session (undergraduate level)

Selected Publications and author role:

S. Phark,Y. Chen, B. Hong, Y. Wang, M. Haze, J. Kim, Y. Bae, A. J. Heinrich, and C. Wolf: Double resonance spectroscopy of coupled electron spins on a surface, Accepted in ACS Nano, (**2023**)

> Co-corresponding author and lead theory author, performed simulations of an open-quantum system of coupled spins

J. Kim, K. Noh, Y. Chen, F. Donati, A.J. Heinrich, C. Wolf, and Y. Bae: Anisotropic hyperfine interaction of surface-adsorbed single atoms, **Nano Letters**, (**2022**)

> Co-corresponding and lead theory author. Ab initio calculations of the hyperfine interaction and origin of their anisotropy

X. Zhang, C. Wolf, Y. Wang, H. Aubin, T. Bilgeri, P. Willke, A. J. Heinrich and T. Choi: Electron Spin Resonance of Single Molecules and Magnetic Interaction through Ligands**, Nature Chemistry** 14, 59-65 (**2022**)

> Lead theory author: developed model for ligand-mediated exchange mechanism based on DFT calculations

A. Singha, D. Sostina, C. Wolf, *et al*.: Mapping Orbital-Resolved Magnetism in Single Lanthanide Atoms, **ACS Nano**, 15, 16162-16171 (**2021**)

> Co-lead author and lead theory author: explanation of the multi-valent charge state of Gd on thin insulating layers based on DFT

C. Wolf, F. Delgado, J. Reina, N. Lorente: Efficient ab initio multiplet calculations for magnetic adatoms on MgO, **The Journal of Physical Chemistry A**, 124, 2318-2327 (**2020**)

First author, leading method development related to mean-field calculations and localized basis set generation

Selected Talks and Posters:

C. Wolf, "Towards full quantum-coherent control of coupled electron spins on a surface", Invited Seminar, TU Wien (Host U. Diebold), 2023/05

C. Wolf, "A Qubit Platform Assembled Atom-by-Atom on a Surface", Contributed Talk, QUANTUMatter2023, Madrid, Spain, 2023/05

C. Wolf, "Towards full quantum-coherent control of coupled electron spins on a surface", Invited Seminar, Fritz Haber Institute Berlin, Germany, 2023/04

C. Wolf, "Surface spins as quantum bits - a simulation perspective", Contribute talk, DPG 2023 Spring Meeting (2023/03)

C. Wolf, "Quantifying super-exchange of molecular dimers using ESR in an STM", Invited talk, KPS 2022 fall meeting (2022/10)

C. Wolf, "Electron-spin resonance on surface spins: recent advances and insights", Invited seminar, FJ Julich-PG1 (2022/09)

C. Wolf, "Electron spin resonance of iron-phthalocyanine molecules on a surface", Contributed talk, DPG 2022 spring meeting (2022/09)

C. Wolf, "Coherent control of individual iron-phthalocyanine molecules on a surface" Poster, MolQuest, Ascona, Switzerland (2022/08)

C. Wolf, "Electron spin resonance of individual iron-phthalocyanine molecules on a surface" Poster, ACS Spring Meeting, San Diego, USA (online, 2022/03)

C. Wolf, "Electron-electron double resonance in an ESR-STM", Invited Talk, KPS Spring meeting (online, 2022/03)

C. Wolf, "Electron spin resonance of iron-phthalocyanine molecules on a surface", Invited Talk, ICAMD 2021, Jeju, South Korea (2021/12)

C. Wolf, "Open Quantum System Model of Electron-Electron Double Resonance of Engineered Atomic Structures on a Surface in an STM", Poster, WE-Heraeus-Seminar, Bad Honnef, Germany (2021/11)

C. Wolf, N. Lorente, "Theoretical understanding of electron spin resonance", Invited Talk, Spins on Surfaces 2, San Sebastian, Spain (2018/09)

Full record of publications:

Total number of citations: 5997, i10-index: 30, h-index: 23 (Google scholar, March 2023)

No.	Publication Title	Number of Authors	Role	Publication Date	IF	Journal
42	Double resonance spectroscopy of coupled electron spins on a surface	9	Joint corresponding	Accepted	14.588	ACS, ACS nano
41	The Influence of the Magnetic Tip on Hetero-dimers in ESR-STM	7	Joint	Submitted	14.588	ACS, ACS nano
40	Many-body non-equilibrium effects in all-electric electron spin resonance	3	Joint corresponding	2023/05	3.908	APS, Physical Review B
39	Erbium and thulium on MgO (100)/Ag (100) as candidates for single atom qubits	13	joint	2023/01	3.908	APS, Physical Review B
38	Anisotropic hyperfine interaction of surface-adsorbed single atoms	7	Joint Corresponding	2022/11	11.238	ACS, Nano Letters
37	Template-Directed Long-Range Ordering of Vanadyl-Phthalocyanine 2D Spin Architecture	11	Joint Corresponding	2023/01	11.684	RSC, Nanoscale Horizons
36	Electron Spin Resonance of Single Molecules and Magnetic Interaction through Ligands	8	Joint	2022/01	24.427	Nature Chemistry
35	Coherent Spin Control of Single Molecules on a Surface	8	Joint	2021/11	14.588	ACS, ACS nano
34	Spin resonance amplitude and frequency of a single atom on a surface in a vector magnetic field	13	Joint	2021/11	4.036	APS, Physical Review B
33	Correlation between Electronic Configuration and Magnetic Stability in Dysprosium Single Atom Magnets	16	Joint	2021/09	11.238	ACS, Nano Letters
32	Mapping Orbital-Resolved Magnetism in Single Lanthanide Atoms	16	Joint Lead	2021/09	14.588	ACS, ACS nano
31	Atomic-scale intermolecular interaction of hydrogen with a single VOPc molecule on the Au (111) surface	5	Joint	2021/01	3.267	RSC, RSC Advances
30	Probing Magnetism in Artificial Metal–Organic Complexes Using Electronic Spin Relaxometry	8	Joint	2020/06	6.475	ACS, The Journal of Physical Chemistry Letters
29	Growth of Multilayer Graphene with a Built-in Vertical Electric Field	9	Joint	2020/05	9.811	ACS, Chemistry of Materials
28	Efficient ab initio multiplet calculations for magnetic adatoms on MgO	4	Primary	2020/02	2.6	ACS, The Journal of Physical Chemistry A

27	Cotunneling mechanism for all-electrical electron spin resonance of single adsorbed atoms	4	Joint	2019/07	4.036	APS, Physical Review B
26	Efficient Perovskite Light-Emitting Diodes Using Polycrystalline Core–Shell-Mimicked Nanograins	11	Joint	2019/05	18.81	Wiley, Advanced Functional Materials
25	Fine control of perovskite crystallization and reducing luminescence quenching using self-doped polyaniline hole injection layer for efficient perovskite light-emitting diodes	12	Joint	2019/02	18.81	Wiley, Advanced Functional Materials
24	Increased luminescent efficiency of perovskite light emitting diodes based on modified two-step deposition method providing gradient concentration	6	Joint	2018/11	5.096	APL, APL Materials
23	Improving the stability of metal halide perovskite materials and light-emitting diodes	5	Joint	2018/10	30.85	Wiley, Advanced Materials
22	Charge carrier recombination and ion migration in metal-halide perovskite nanoparticle films for efficient light-emitting diodes	4	Joint	2018/10	17.881	Elsevier, Nano Energy
21	Ultrasensitive artificial synapse based on conjugated polyelectrolyte	16	Joint	2018/06	17.881	Elsevier, Nano Energy
20	High-efficiency polycrystalline perovskite light-emitting diodes based on mixed cations	12	Joint	2018/03	14.588	ACS, ACS nano
19	Exciton and lattice dynamics in low-temperature processable CsPbBr3 thin-films	2	Primary	2018/30	7.01	Elsevier, Materials today energy
18	Unravelling additive-based nanocrystal pinning for high efficiency organic-inorganic halide perovskite light-emitting diodes	10	Joint	2017/12	17.881	Elsevier, Nano Energy
17	Polaronic charge carrier–lattice interactions in lead halide perovskites	4	Primary	2017/10	8.928	Wiley, ChemSusChem
16	Ultrapure green light-emitting diodes using two-dimensional formamidinium perovskites: Achieving recommendation 2020 color coordinates	12	Joint	2017/09	11.238	ACS, Nano letters
15	High-Efficiency Solution-Processed Inorganic Metal Halide Perovskite Light-Emitting Diodes	9	Joint	2017/08	30.85	Wiley, Advanced Materials

14	High efficiency perovskite light-emitting diodes of ligand-engineered colloidal formamidinium lead bromide nanoparticles	8	Joint	2017/08	17.881	Elsevier, Nano Energy
13	Highly efficient light-emitting diodes of colloidal metal–halide perovskite nanocrystals beyond quantum size	12	Joint	2017/07	14.588	ACS, ACS nano
12	Structural and Thermal Disorder of Solution-Processed CH3NH3PbBr3 Hybrid Perovskite Thin Films	3	Primary	2017/03	9.229	ACS, applied materials & interfaces
11	Efficient visible quasi-2D perovskite light-emitting diodes	8	Joint	2016/09	30.85	Wiley, Advanced Materials
10	Organometal halide perovskite artificial synapses	7	Joint	2016/07	30.85	Wiley, Advanced Materials
9	On-Fabrication Solid-State N-Doping of Graphene by an Electron-Transporting Metal Oxide Layer for Efficient Inverted Organic Solar Cells	12	Joint	2016/06	29.368	Wiley, Advanced Energy Materials
8	Highly Efficient, Simplified, Solution-Processed Thermally Activated Delayed-Fluorescence Organic Light-Emitting Diodes	5	Joint	2016/01	30.85	Wiley, Advanced Materials
7	Overcoming the electroluminescence efficiency limitations of perovskite light-emitting diodes	13	Joint	2015/12	41.84	AAAS, Science
6	Resistive switching based on filaments in metal/PMMA/metal thin film devices	6	Primary	2015/11	1.471	IOP, Japanese Journal of Applied Physics
5	Synergistic effects of doping and thermal treatment on organic semiconducting nanowires	4	Joint	2015/09	9.229	ACS, applied materials & interfaces
4	Monolithically integrated organic resistive switches for luminance and emission color manipulation in polymer light emitting diodes	5	Joint	2015/09	3.791	APS, Applied physics letters
3	Planar CH3NH3PbI3 Perovskite Solar Cells with Constant 17.2% Average Power Conversion Efficiency Irrespective of the Scan Rate	11	Joint	2015/06	30.85	Wiley, Advanced Materials
2	Inkjet-Printed Resistive Switching Memory Based on Organic Dielectric Materials: From Single Elements to Array Technology	9	Joint	2015/02	7.295	Wiley, Advanced Electronic Materials
1	Organic Non-Volatile Resistive Photo-Switches for Flexible Image Detector Arrays	4	Joint	2015/02	30.85	Wiley, Advanced Materials