

# DR. BENEDIKT P. KLEIN - Curriculum Vitae

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## PROFESSIONAL EXPERIENCE

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| 2023 -      | POSTDOCTORAL RESEARCHER, <i>Korea Basic Science Institute</i><br>Material analysis using X-ray photoelectron spectroscopy   |
| 2021 - 2023 | WALTER-BENJAMIN RESEARCH FELLOW (DFG)<br><i>University of Warwick and Diamond Light Source</i><br>Development of graphene-based substrates for single-atom catalysis, using a surface science approach combined with quantum chemistry calculations |
| 2020 - 2021 | RESEARCH FELLOW, <i>University of Warwick</i><br>Research in theoretical chemistry, computational simulation of electron spectroscopy   |
| 2015 - 2019 | RESEARCH ASSISTANT, <i>Philipps-Universität Marburg</i><br>Research and teaching duties in the Collaborative Research Centre 1083, "Structure and Dynamics of Internal Interfaces"  |
| 2012 - 2015 | TEACHING ASSISTANT, <i>Philipps-Universität Marburg</i><br>Conducting of seminars and lab courses in mathematics and physical chemistry   |

## EDUCATION

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| 2016 - 2019 | PHD STUDIES IN CHEMISTRY, <i>Philipps-Universität Marburg</i><br>Research in the group of Prof. M. Gottfried, investigation of metal-organic interfaces<br>Development of scientific UHV instruments<br>Thesis: "The Surface Chemical Bond of Non-alternant Aromatic Molecules on Metal Surfaces"<br>Degree: Dr. rer. nat., Grade: <i>summa cum laude</i> ("excellent") |
| 2012 - 2016 | MASTER OF SCIENCE IN CHEMISTRY, <i>Philipps-Universität Marburg</i><br>Focus: Physical, theoretical and inorganic chemistry<br>Thesis: "Untersuchungen zur Adsorption von Azulen und Naphthalin auf Cu(111) und Ag(111)"<br>Overall grade: "excellent"  |
| 2009 - 2012 | BACHELOR OF SCIENCE IN CHEMISTRY, <i>Philipps-Universität Marburg</i><br>Focus: Physical and theoretical chemistry<br>Thesis: "Charakterisierung eines Magnesiumatomstrahls", overall grade: "very good"  |

## MILITARY SERVICE

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| 2008 - 2009 | MILITARY SERVICE, <i>345th Regiment of Artillery, German Army</i> |
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## HONOURS AND AWARDS

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| 2020        | AWARD FOR THE BEST PHD THESIS OF 2019<br>Philipps-Universität Marburg  |
| 2017        | BEST POSTER AWARD, <i>Interdisciplinary and Intercultural Summer School</i><br>Tongji University Shanghai and Philipps-Universität Marburg |
| 2010 - 2015 | FULLY FUNDED SCHOLARSHIP<br>Studienstiftung des deutschen Volkes   |

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## SELECTED PUBLICATIONS

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- 1 **B.P. Klein**, M.A. Stoodley, M. Edmondson, L.A. Rochford, M. Walker, L. Sattler, S.M. Weber, G. Hilt, L.B.S. Williams, T.-L. Lee, A. Saywell, R.J. Maurer, and D.A. Duncan, *Using polycyclic aromatic hydrocarbons for graphene growth on Cu(111) under ultra-high vacuum*, Appl. Phys. Lett **2022**, 121, 191603. DOI: [10.1063/5.0122914](https://doi.org/10.1063/5.0122914).
- 2 **B.P. Klein**, A. Ihle, S.R. Kachel, L. Ruppenthal, S.J. Hall, L.E. Sattler, S.M. Weber, J. Herritsch, A. Jaegermann, D. Ebeling, R.J. Maurer, G. Hilt, R. Tonner-Zech, A. Schirmeisen, J.M. Gottfried, *Topological Stone Wales Defects Enhance Bonding and Electronic Coupling at the Graphene/Metal Interface*, ACS Nano **2022**, 16, 11979-11987. DOI: [10.1002/cphc.202100222](https://doi.org/10.1002/cphc.202100222).
- 3 **B.P. Klein**, S.J. Hall, R.J. Maurer, *The Nuts and Bolts of Ab-Initio Core-Hole Simulations for K-shell X-Ray Photoemission and Absorption Spectra*, J. Phys. Condens. Matter **2021**, 23, 154005. DOI: [10.1088/1361-648X/abdf00](https://doi.org/10.1088/1361-648X/abdf00).
- 4 **B.P. Klein**, S.E. Harman, L. Ruppenthal, G.M. Ruehl, S.J. Hall, S.J. Carey, J. Herritsch, M. Schmid, R.J. Maurer, R. Tonner, C.T. Campbell, J.M. Gottfried, *Enhanced Bonding of Pentagon-Heptagon Defects in Graphene to Metal Surfaces: Insights from the Adsorption of Azulene and Naphthalene to Pt(111)*, Chem. Mater. **2020**, 32, 1041-1053. DOI: [10.1021/acs.chemmater.9b03744](https://doi.org/10.1021/acs.chemmater.9b03744).
- 5 **B.P. Klein**, J.M. Morbec, M. Franke, K.K. Greulich, M. Sachs, S. Parhizkar, F.C. Bocquet, M. Schmid, S.J. Hall, R.J. Maurer, B. Meyer, R. Tonner, C. Kumpf, P. Kratzer, J.M. Gottfried, *Molecule-Metal Bond of Alternant versus Nonalternant Aromatic Isomers on Coinage Metal Surfaces: Naphthalene versus Azulene on Ag(111) and Cu(111)*, J. Phys. Chem. C **2019**, 123, 29219-29230. DOI: [10.1021/acs.jpcc.9b08824](https://doi.org/10.1021/acs.jpcc.9b08824).
- 6 **B.P. Klein**, N.J. van der Heijden, S.R. Kachel, M. Franke, C.K. Krug, K.K. Greulich, L. Ruppenthal, P. Müller, P. Rosenow, S. Parhizkar, F. C. Bocquet, M. Schmid, W. Hieringer, R. J. Maurer, R. Tonner, C. Kumpf, I. Swart, J. M. Gottfried, *Molecular Topology and the Surface Chemical Bond: Alternant Versus Nonalternant Aromatic Systems as Functional Structural Elements*, Phys. Rev. X **2019**, 9, 011030. DOI: [10.1103/PhysRevX.9.011030](https://doi.org/10.1103/PhysRevX.9.011030).