

Paul Jerabek

Group Leader Computational Materials Design
Deputy Head of Department of Materials Design

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Scholar profile

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Helmholtz-Zentrum Hereon, Max-Planck-Straße 1, 21502 Geesthacht

Education

- Dec 2010 – Sep 2014 **Dr. rer. nat.**, *Philipps-Universität Marburg*
Thesis: *Clusterartige und hochkoordinierte Metallkomplexe*
- Jun 2010 – Nov 2010 **Dipl.-Chem.**, *Philipps-Universität Marburg*
Thesis: *Bindungstheoretische Untersuchungen der Systeme des Typs YE-X-EY*
- Oct 2005 – Jun 2010 **Studies of Chemistry**, *Philipps-Universität Marburg*

Professional experience

- Sep 2022 – present **Deputy Head of Department of Materials Design**, *Helmholtz-Zentrum Hereon*
Department administration and representation, third-party funding acquisition, research strategy planning, digital transformation.
- Oct 2021 – present **Co-Leader, German-New Zealand Green Hydrogen Centre (He Honoka Hauwai)**, *Helmholtz-Zentrum Hereon / University of Otago*
Administration and representation, strategic planning, networking, funding acquisition, event organization.
- Sep 2019 – present **Group Leader “Metal Hydride Modeling”**, *Helmholtz-Zentrum Hereon*
First-principles molecular dynamics, CALPHAD and phase-field simulations for the characterization and optimization of novel metal hydride materials for large-scale hydrogen storage. Close collaborations with Lawrence Livermore National Laboratory (USA) and the University of Otago (New Zealand).
- Jul 2018 – Aug 2019 **Humboldt Return Fellow**, *Max-Planck-Institut für Kohlenforschung*
Theoretical investigation of physical properties of organesson; substituent and solvent effects on switching temperature in Fe(II) spin-crossover complexes; reaction mechanism exploration for asymmetrical, homogeneous catalysis; bonding situation and electronic properties of pincer complexes.
- Dec 2017 – Jun 2018 **Postdoctoral Research Assistant**, *Massey University*
Monte-Carlo melting simulations of heavy and superheavy elements; first-principles molecular dynamics simulations of coinage metals in liquid and solid phase; highly accurate calculations of atomic polarizabilities.
- Dec 2015 – Nov 2017 **Feodor Lynen Research Fellow**, *Massey University*
Photochemistry of small molecules in different environments; influence of relativistic and solvent effects on atomic and molecular bonding properties; development of highly accurate ab-initio many-body potentials for heavy and superheavy elements.
- Dec 2014 – Nov 2015 **Postdoctoral Research Assistant**, *Philipps-Universität Marburg*
Method development (C) for core electron spectroscopy of organic molecules on surfaces; density functional theory based investigation of transition metal clusters and complexes.

Dec 2010 – Nov 2014	Research Assistant, <i>Philipps-Universität Marburg</i> Quantum chemical investigation of main-group and transition metal compounds in collaboration with experimental groups in Bochum, München, Göttingen, Dresden, Münster and San Diego. Redesign of the lab course in Theoretical Chemistry.
Jan 2007 – Dec 2010	Student Assistant, <i>Philipps-Universität Marburg</i> Supervision of lab courses in Physical Chemistry and Chemistry for Medical Students.

Third-party funding

2024	Sustainable TiFe Generation from Secondary Sources BMBF (Germany) Principal Investigator 1.5 M€ 3 years
2024	HIDA Visiting Researcher Grant (with S. Faouri) Helmholtz Association Host 10 k€ 2 months
2023	HIDA Visiting Researcher Grant (with A. Rowberg) Helmholtz Association Host 15 k€ 3 months
2022	Generating Hydrogen Storage Materials from New Zealand Resources BMBF (Germany) Coordinator 400 k€ 3 years
2021	Establishing a German-New Zealand Research Centre for Green Hydrogen BMBF (Germany) Coordinator 760 k€ 5 years
2021	HIDA Visiting Scientist Grant (with M. Selzer) Helmholtz Association Fellow 10 k€ 3 months
2017	Humboldt Return Fellowship Alexander von Humboldt Foundation Fellow 47 k€ 1 year
2016	Computation of highly accurate interatomic potentials of heavy and superheavy elements New Zealand eScience Infrastructure (NeSI) Principal Investigator 117 k€ 1.5 years
2014	Hochpräzise quantenchemische Simulationen von atomaren und molekularen Phasen unter extremen Bedingungen Alexander von Humboldt Foundation Fellow 85 k€ 2 years

Conference organization

2025	E-MRS Fall Meeting 2025 — Symposium A Co-organizer, Warsaw, Poland
2024	E-MRS Fall Meeting 2024 — Symposium C: Sustainable materials for chemical and electrochemical energy storage II Main organizer, Warsaw, Poland
2023	Inaugural New Zealand Hydrogen Symposium Co-organizer, Dunedin, New Zealand
2015	Bonding Analysis Workshop Conceptualization and main organizer, Marburg, Germany

Teaching

2025 SoSe	Hydrogen Technology Co-lecturer, Technische Universität Hamburg (TUHH), Hamburg
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2023 – present	Lectureship Lecturer, Technische Hochschule Mittelhessen, Gießen
2019 – 2019	Knowledge for Tomorrow – Cooperative Research Projects in Sub-Saharan Africa (Volkswagen-Stiftung) Tutor, University of Mauritius, Reduit
2014 – 2019	Hands-on workshops on electronic structure methods Workshop lecturer, Various universities, Hyderabad, Dunedin, Denton, Mariapfarr, Mauritius
2010 – 2014	Practical course in Theoretical Chemistry Teaching assistant, Philipps-Universität Marburg, Marburg
2007 – 2010	Physical Chemistry and Chemistry for Medical Students Student assistant, Philipps-Universität Marburg, Marburg

Talks and posters

May 2025	German-New Zealand WTZ Meeting 2025 , Wellington, New Zealand Invited Talk
Feb 2025	11th International Conference on Advanced Materials and Nanotechnology (AMN11) , Christchurch, New Zealand Invited Talk
Jul 2024	New Zealand-Germany Energy Dialogue 2024 , Berlin, Wellington, Germany, New Zealand Invited Talk
Feb 2023	10th International Conference on Advanced Materials and Nanotechnology (AMN10) , Rotorua, New Zealand Invited Talk
Jul 2018	18th International Conference on Computational and Mathematical Methods in Science and Engineering (CMMSE-2018) , Rota, Spain Invited Talk
Jul 2016	16th International Conference on Computational and Mathematical Methods in Science and Engineering (CMMSE-2016) , Rota, Spain Invited Talk
Mar 2024	German Physical Society (DPG) Spring Meeting 2024 , Berlin, Germany Contributed Talk
Jan 2024	2nd New Zealand Hydrogen Symposium (NZHS-2) , Wellington, New Zealand Contributed Talk
Mar 2023	German Physical Society (DPG) Spring Meeting 2023 , Dresden, Germany Contributed Talk
Sep 2022	European Materials Research Society (E-MRS) Fall Meeting 2022 , Warsaw, Poland Contributed Talk
Mar 2019	Chemiedozententagung 2019 , Koblenz, Germany Contributed Talk
Nov 2017	17th Biennial Symposium of the Australian and New Zealand Associations of von Humboldt Fellows , Wellington, New Zealand Contributed Talk
Sep 2017	12th International Conference on Relativistic Effects in Heavy-Element Chemistry and Physics (REHE) , Marburg, Germany Contributed Talk

Aug 2016	New Zealand Institute of Chemistry Conference (NZIC-16) , Queenstown, New Zealand Contributed Talk
May 2024	18th International Symposium of Metal-Hydrogen Systems (MH 2024) , Saint-Malo, France Poster
Sep 2018	54th Symposium on Theoretical Chemistry (STC) , Halle (Saale), Germany Poster
Aug 2017	11th World Association of Theoretical and Computational Chemists (WATOC) , Munich, Germany Poster
Jul 2016	9th Congress of the International Society for Theoretical Chemical Physics (ISTCP IX) , Grand Forks (ND), USA Poster
Sep 2015	51st Symposium on Theoretical Chemistry (STC) , Postdam, Germany Poster
Sep 2013	49th Symposium on Theoretical Chemistry (STC) , Erlangen, Germany Poster
Sep 2012	48th Symposium on Theoretical Chemistry (STC) , Karlsruhe, Germany Poster
Oct 2011	Modeling of Molecular Properties Conference (MolMod) , Heidelberg, Germany Poster
Jul 2011	9th World Association of Theoretical and Computational Chemists (WATOC) , Santiago de Compostela, Spain Poster
Sep 2010	46th Symposium on Theoretical Chemistry (STC) , Münster, Germany Poster
Feb 2025	University of Waikato , Hamilton, New Zealand Invited Seminar
Jun 2024	University of Hamburg , Hamburg, Germany Invited Seminar
Feb 2024	Massey University , Auckland, New Zealand Invited Seminar
Feb 2024	University of Waikato , Hamilton, New Zealand Invited Seminar
Mar 2023	Massey University , Auckland, New Zealand Invited Seminar
Mar 2023	University of Auckland , Auckland, New Zealand Invited Seminar
Dec 2021	Karlsruhe Institute of Technology (KIT) , Karlsruhe, Germany Invited Seminar
May 2019	Helmholtz-Zentrum für Material- und Küstenforschung , Geesthacht, Germany Invited Seminar
Apr 2019	Universität Graz , Graz, Austria Invited Seminar
Feb 2019	Technische Universität Berlin , Berlin, Germany Invited Seminar

Jan 2019	GSI Helmholtzzentrum für Schwerionenforschung , Darmstadt, Germany Invited Seminar
Feb 2018	University of Otago , Dunedin, New Zealand Invited Seminar
Jun 2017	University of Otago , Dunedin, New Zealand Invited Seminar
Jul 2016	University of North Texas , Denton (TX), USA Invited Seminar
Oct 2019	Summer School/Workshop on Computational Chemistry “Knowledge for Tomorrow – Cooperative Research Projects in Sub-Saharan Africa” , Reduit, Mauritius Workshop Lecture
Mar 2019	XIIth Workshop on Modern Methods in Quantum Chemistry , MariaPfarr, Austria Workshop Lecture
Dec 2017	University of Otago , Dunedin, New Zealand Workshop Lecture
Jul 2016	University of North Texas , Denton (TX), USA Workshop Lecture
Jan 2014	MCBR Winter School , Hyderabad, India Workshop Lecture

Peer-reviewed journal articles

70. E. Pericoli, V. Ferretti, E. Alvares, **P. Jerabek**, C. Pistidda, L. Pasquini, Evaluation of the synergetic effects of Ni and Cr in $\text{TiFe}(1-x-y)\text{Cr}_x\text{Ni}_y$ for enhanced hydriding thermodynamics, *Adv. Energy Sustain. Res.* **2026**, 7, e70243.
69. J.-E. Ahrens, **P. Jerabek**, L. Vondung, Relativistic effects are crucial for uraniumphosphorus bonding - a DFT study of cyclopentadienyluranium-phosphine complexes, *Mol. Phys.* **2026**, e2611400.
68. A. J. E. Rowberg, S. Kang, K. Sellschopp, **P. Jerabek**, T. W. Heo, B. C. Wood, Role of Elemental Substitution on Hydrogen Incorporation in Characteristic Ti-Fe-Based Oxides, *ACS Appl. Energy Mater.* **2026**, 9, 1242–1253.
67. Y. Shang, A. Santhosh, **P. Jerabek**, T. Klassen, C. Pistidda, Leveraging atomic disorder to modulate hydrogen storage thermodynamics in compositionally complex intermetallics, *Interdiscip. Mater.* **2026**, 0, 1-13.
66. L. Dinachandran, E. Alvares, K. Sellschopp, T. Klassen, **P. Jerabek**, A. L. Garden, Predicting hydrogen storage capacity loss of Si-containing FeTi alloys through ab initio thermodynamic modeling, *Acta Mater.* **2025**, 301, 121514.
65. A. Chandran, A. Santhosh, **P. Jerabek**, R. C. Aydin, C. J. Cyron, TiAlNb alloy interatomic potentials - comparing passive and active machine learning techniques with MTP and DeepMD, *Front. Mater.* **2025**, 12.
64. Y. Shang, A. Santhosh, M. Ante, L. Wimbert, **P. Jerabek**, T. Schupp, T. Klassen, C. Pistidda, Low-temperature regeneration of metal hydride after impurity gas exposure, *Acta Mater.* **2025**, 298, 121398.
63. T. T. Le, K. Sellschopp, F. Murgia, A. L. Garden, S. Bordignon, J. P. Embs, M. R. Chierotti, A. Schökel, F. Karimi, **P. Jerabek**, T. Klassen, C. Pistidda, High Ionic Conduction in Rb-

- and Cs-Mixed Cation Amide for Energy Storage, *Small* **2025**, 2502943.
62. E. Alvares, A. J. E. Rowberg, K. Sellschopp, B. C. Wood, T. Klassen, **P. Jerabek**, C. Pistidda, A Thermodynamic Approach to Model Multicomponent FeTi-based Alloys for Hydrogen Storage, *Scr. Mater.* **2025**, 259, 116516.
 61. E. Alvares, K. Sellschopp, B. Wang, S. Kang, T. Klassen, T. W. Heo, T. Klassen, **P. Jerabek**, C. Pistidda, Multiscale Modeling the FeTi Metal-Hydride Interphase Boundaries – Quantification of Decoupled Chemo-Mechanical Energies, *npj Comput. Mater.* **2024**, 10, 249.
 60. A. Chandran, A. Santhosh, C. Pistidda, **P. Jerabek**, R. Aydin, C. J. Cyron, Comparative analysis of ternary TiAlNb interatomic potentials - moment tensor vs. deep learning approaches, *Front. Mater.* **2024**, 11, 1466793.
 59. P. Hannappel, E. Alvares, F. Heubner, C. Pistidda, **P. Jerabek**, T. Weißgärber, Thermodynamic assessment of the Ce-H and CeNi₅-H system, *Calphad* **2024**, 85, 102701.
 58. M. Robb, L. Bondi, S. Rodriguez-Jimenez, A. Garden, **P. Jerabek**, S. Brooker, Predictable Electronic Tuning of FeII versus RuII Complexes via Choice of Azine Donor - An Electrochemical and Theoretical Study, *Dalton Trans.* **2024**, 53, 1999-2007.
 57. A. Robles-Navarro, **P. Jerabek**, P. Schwerdtfeger, Tipping the balance between the bcc and fcc phase within the alkali and coinage metal groups, *Angew. Chem. Int. Ed.* **2024**, 63, e202313679.
 56. Y. Shang, A. Santhosh, **P. Jerabek**, T. Klassen, C. Pistidda, First-principles study on interfacial property in MgB₂-based reactive hydride composites, *Scr. Mater.* **2024**, 240, 115837.
 55. M. Ghazanfari, K. Siemensmeyer, A. Santhosh, J. Vrijmoed, M. Tallu, S. Dehnen, **P. Jerabek**, G. Thiele, Low-Cost, Multifunctional, and Sustainable Sodium Sulfido Ferrate(II), *Inorg. Chem.* **2023**, 62, 15358-15366.
 54. Y. Shang, Z. Lei, E. Alvares, S. Garroni, R. Dore, M. Rustici, S. Enzo, A. Schökel, Y. Shi, **P. Jerabek**, Z. Lu, T. Klassen, C. Pistidda, Ultra-lightweight compositionally complex alloys with large ambient-temperature hydrogen storage capacity, *Mater. Today* **2023**, 67, 113-126.
 53. A. Santhosh, S. Kang, N. Keilbart, B. C. Wood, T. Klassen, **P. Jerabek**, M. Dornheim, Influence of near-surface oxide layers on TiFe hydrogenation - Mechanistic insights and implications for hydrogen storage applications, *J. Mater. Chem. A* **2023**, 11, 18776-18789.
 52. T.-T. Le, A. Santhosh, S. Bordignon, M. R. Chierotti, **P. Jerabek**, T. Klassen, C. Pistidda, Experimental and Computational Studies on the Formation of Mixed Amide-Hydride Solid Solutions for CsNH₂-CsH System, *Results in Engineering* **2023**, 17, 100895.
 51. L. Pasquini, K. Sakaki, E. Akiba, **P. Jerabek** et al., Magnesium- and intermetallic alloys-based hydrides for energy storage: modelling, synthesis and properties, *Prog. Energy* **2022**, 4, 32007.
 50. **P. Jerabek**, A. Santhosh, P. Schwerdtfeger, Relativistic Effects Stabilize Unusual Gold(II) Sulfate Structure via Aurophilic Interactions, *Inorg. Chem.* **2022**, 61, 13077-13084.
 49. **P. Jerabek**, A. Burrows, P. Schwerdtfeger, Solving a problem with a single parameter: A smooth bcc to fcc phase transition for metallic lithium, *Chem. Commun.* **2022**, 58, 13369-13372.

48. M. R. Ghazanfari, L. Vittadello, D. Al-Sabbagh, A. Santhosh, C. Frankcom, F. Fuß, C. A. von Randow, K. Siemensmeyer, J. C. Vrijmoed, F. Emmerling, **P. Jerabek**, M. Imlau, G. Thiele, Remarkable Infrared Nonlinear Optical, Dielectric, and Strong Diamagnetic Characteristics of Semiconducting K₃[BiS₃], *J. Phys. Chem. Lett.* **2022**, *13*, 6987–6993.
47. M. R. Ghazanfari, A. Santhosh, J. C. Vrijmoed, K. Siemensmeyer, B. Peters, S. Dehnen, **P. Jerabek**, G. Thiele, Large-scale synthesis of mixed valence K₃[Fe₂S₄] with high dielectric and ferrimagnetic characteristics, *RSC Adv.* **2022**, *12*, 30514–30521.
46. M. R. Ghazanfari, A. Santhosh, K. Siemensmeyer, F. Fuß, L. Staab, J. C. Vrijmoed, B. Peters, M. Liesegang, S. Dehnen, O. Oeckler, **P. Jerabek**, G. Thiele, Large Exchange Bias, High Dielectric Constant, and Outstanding Ionic Conductivity in a Single-Phase Spin Glass, *Adv. Electron. Mater.* **2022**, *8*, 2200483.
45. E. Florez, O. R. Smits, J.-M. Mewes, **P. Jerabek**, P. Schwerdtfeger, From the gas phase to the solid state: The chemical bonding in the superheavy element flerovium, *J. Chem. Phys.* **2022**, *157*, 64304.
44. D. M. Dreistadt, L. Thi-Thu, G. Capurso, J. M. Bellosta von Colbe, A. Santhosh, C. Pistidda, N. Scharnagl, H. Ovari, C. Milanese, **P. Jerabek**, T. Klassen, J. Jepsen, An Effective Activation Method for Industrially Produced TiFeMn Powder for Hydrogen Storage, *J. Alloys Compd.* **2022**, *919*, 165847.
43. L. Bondi, A. L. Garden, F. Totti, **P. Jerabek**, S. Brooker, Quantitative assessment of ligand substituent effects on σ - and π -contributions to Fe-N bonds in spin crossover FeII complexes, *Chem. Eur. J.* **2022**, *28*, e202104314.
42. E. Alvares, **P. Jerabek**, Y. Shang, A. Santhosh, C. Pistidda, T. W. Heo, B. Sundman, M. Dornheim, Modeling the thermodynamics of the FeTi hydrogenation under para-equilibrium: An ab-initio and experimental study, *Calphad* **2022**, *77*, 102426.
41. C. Pistidda, A. Santhosh, **P. Jerabek**, Y. Shang, A. Girella, C. Milanese, M. Dore, S. Garroni, S. Bordignon, M. R. Chierotti, T. Klassen, M. Dornheim, Hydrogenation via a low energy mechanochemical approach: The MgB₂ case, *J. Phys. Energy* **2021**, *3*, 44001.
40. O. R. Smits, J. Mewes, **P. Jerabek**, P. Schwerdtfeger, Oganesson: A Noble Gas Element That Is Neither Noble Nor a Gas, *Angew. Chem. Int. Ed.* **2020**, *59*, 23636–23640.
39. O. R. Smits, **P. Jerabek**, E. Pahl, P. Schwerdtfeger, First-principles melting of krypton and xenon based on many-body relativistic coupled-cluster interaction potentials, *Phys. Rev. B* **2020**, *101*, 104103.
38. M. Buchsteiner, L. Martinez-Rodriguez, **P. Jerabek**, I. Pozo, M. Patzer, N. Nöthling, C. W. Lehmann, A. Fürstner, Catalytic Asymmetric Fluorination of Copper Carbene Complexes: Preparative Advances and a Mechanistic Rationale, *Chem. Eur. J.* **2020**, *26*, 2509–2515.
37. L. Bondi, A. L. Garden, **P. Jerabek**, F. Totti, S. Brooker, Quantitative and Chemically Intuitive Evaluation of the Nature of M–L Bonds in Paramagnetic Compounds: Application of EDA-NOCV Theory to Spin Crossover Complexes, *Chem. Eur. J.* **2020**, *26*, 13677–13685.
36. L. Vondung, **P. Jerabek**, R. Langer, Ligands Based on Phosphine-Stabilized Aluminum(I), Boron(I), and Carbon(0), *Chem. Eur. J.* **2019**, *25*, 3068–3076.
35. J.-M. Mewes, **P. Jerabek**, O. R. Smits, P. Schwerdtfeger, Oganesson Is a Semiconductor: On the Relativistic Band-Gap Narrowing in the Heaviest Noble-Gas Solids, *Angew. Chem. Int. Ed.* **2019**, *58*, 14260–14264.

34. **P. Jerabek**, O. R. Smits, J.-M. Mewes, K. A. Peterson, P. Schwerdtfeger, Solid Oganesson via a Many-Body Interaction Expansion Based on Relativistic Coupled-Cluster Theory and from Plane-Wave Relativistic Density Functional Theory, *J. Phys. Chem. A* **2019**, *123*, 4201–4211.
33. **P. Jerabek**, P. Schwerdtfeger, G. Frenking, Dative and Electron-Sharing Bonding in Transition Metal Compounds, *J. Comput. Chem.* **2019**, *40*, 247–264.
32. O. Smits, **P. Jerabek**, E. Pahl, P. Schwerdtfeger, A Hundred-Year-Old Experiment Re-evaluated: Accurate Ab-Initio Monte-Carlo Simulations of the Melting of Radon, *Angew. Chem. Int. Ed.* **2018**, *57*, 9961–9964.
31. J.-M. Mewes, **P. Jerabek**, D. S. Bohle, P. Schwerdtfeger, The Light-Driven Isomerization of Aqueous Nitrate: A Theoretical Perspective, *ChemPhotoChem* **2018**, *2*, 725–733.
30. **P. Jerabek**, L. Vondung, P. Schwerdtfeger, Tipping the Balance between Ligand and Metal Protonation due to Relativistic Effects: Unusually High Proton Affinity in Gold(I) Pincer Complexes, *Chem. Eur. J.* **2018**, *24*, 6047–6051.
29. **P. Jerabek**, O. Smits, E. Pahl, P. Schwerdtfeger, A relativistic coupled-cluster interaction potential and rovibrational constants for the xenon dimer, *Mol. Phys.* **2018**, *116*, 1–8.
28. **P. Jerabek**, P. Schwerdtfeger, J. K. Nagle, Static dipole polarizability of palladium from relativistic coupled-cluster theory, *Phys. Rev. A* **2018**, *98*, 12508.
27. **P. Jerabek**, B. Schuetrumpf, P. Schwerdtfeger, W. Nazarewicz, Electron and nucleon localization functions of oganesson: Approaching the Thomas-Fermi limit, *Phys. Rev. Lett.* **2018**, *120*, 53001.
26. J. Hornung, J. Weßing, **P. Jerabek**, C. Gemel, A. Pöthig, G. Frenking, R. A. Fischer, Suppressed Phosphine Dissociation by Polarization Effects on the Donor–Acceptor Bonds in [Ni(PEt₃)_{4–n} (ECp*)_n] (E = Al, Ga), *Inorg. Chem.* **2018**, *57*, 12657–12664.
25. **P. Jerabek**, B. von der Esch, H. Schmidbaur, P. Schwerdtfeger, Influence of Relativistic Effects on Bonding Modes in M(II) Dinuclear Complexes (M = Au, Ag, and Cu), *Inorg. Chem.* **2017**, *56*, 14624–14631.
24. Q. Zhang, **P. Jerabek**, M. Chen, M. Zhou, G. Frenking, The Oxygen-Rich Beryllium Oxides BeO₄ and BeO₆, *Angew. Chem. Int. Ed.* **2016**, *55*, 10863–10867.
23. M. Klues, **P. Jerabek**, T. Breuer, M. Oehzelt, K. Hermann, R. Berger, G. Witte, Understanding the F 1s NEXAFS Dichroism in Fluorinated Organic Semiconductors, *J. Phys. Chem. C* **2016**, *120*, 12693–12705.
22. K. Freitag, M. Molon, **P. Jerabek**, K. Dilchert, C. Rösler, R. W. Seidel, C. Gemel, G. Frenking, R. A. Fischer, Zn...Zn interactions at nickel and palladium centers, *Chem. Sci.* **2016**, *7*, 6413–6421.
21. K. Freitag, C. Gemel, **P. Jerabek**, M. I. Oppel, R. W. Seidel, G. Frenking, H. Banh, K. Dilchert, R. A. Fischer, The σ -Aromatic Clusters [Zn₃]⁺ and [Zn₂Cu]: Embryonic Brass, *Angew. Chem. Int. Ed.* **2015**, *54*, 4370–4374.
20. C. Clobes, **P. Jerabek**, I. Nußbruch, G. Frenking, C. von Hähnisch, Stepwise Synthesis of Siloxane-Substituted Oligoarsanes and Structural Investigation of Alkaline Earth Metal Derivatives, *Eur. J. Inorg. Chem.* **2015**, 3264–3273.
19. D. S. Weinberger, N. Amin SK, K. C. Mondal, M. Melaimi, G. Bertrand, A. C. Stückl, H. W. Roesky, B. Dittrich, S. Demeshko, B. Schwederski, W. Kaim, **P. Jerabek**, G.

- Frenking, Isolation of Neutral Mononuclear Copper Complexes Stabilized by Two Cyclic (Alkyl)(amino)carbenes, *J. Am. Chem. Soc.* **2014**, *136*, 6235–6238.
18. A. Puls, **P. Jerabek**, W. Kurashige, M. Molon, T. Bollermann, M. Winter, C. Gemel, Y. Negishi, G. Frenking, R. A. Fischer, A Novel Concept for the Synthesis of Multiply Doped Gold Clusters $[(M@AunM'm)Lk]q+$, *Angew. Chem. Int. Ed.* **2014**, *53*, 4327–4331.
 17. B. Niepötter, R. Herbst-Irmer, D. Kratzert, P. P. Samuel, K. C. Mondal, H. W. Roesky, **P. Jerabek**, G. Frenking, D. Stalke, Experimental Charge Density Study of a Silylone, *Angew. Chem. Int. Ed.* **2014**, *53*, 2766–2770.
 16. M. Molon, C. Gemel, **P. Jerabek**, L. Trombach, G. Frenking, R. A. Fischer, Hume-Rothery Phase-Inspired Metal-Rich Molecules: Cluster Expansion of $[Ni(ZnMe)_6(ZnCp^*)_2]$ by Face Capping with $Ni(0)(\eta(6)\text{-toluene})$ and $Ni(I)(\eta(5)\text{-Cp}^*)$, *Inorg. Chem.* **2014**, *53*, 10403–10411.
 15. **P. Jerabek**, H. W. Roesky, G. Bertrand, G. Frenking, Coinage Metals Binding as Main Group Elements: Structure and Bonding of the Carbene Complexes $[TM(cAAC)_2]$ and $[TM(cAAC)_2]^+$ ($TM = Cu, Ag, Au$), *J. Am. Chem. Soc.* **2014**, *136*, 17123–17135.
 14. **P. Jerabek**, G. Frenking, Comparative bonding analysis of N_2 and P_2 versus tetrahedral N_4 and P_4 , *Theor. Chem. Acc.* **2014**, *133*, 1447–1456.
 13. N. B. Jaufeerally, P. Ramasami, **P. Jerabek**, G. Frenking, Bonding analysis of telluroketones $H_2A=Te$ ($A = C, Si, Ge$), *J. Mol. Mod.* **2014**, *20*, 2433–2440.
 12. K. Freitag, H. Banh, C. Gemel, **P. Jerabek**, G. Frenking, R. A. Fischer, Dizinc Cation $[Zn_2]^+$ Trapped In A Homoleptic Metalloid Coordination Environment Stabilized by Dispersion Forces: $[Zn_2(GaCp^*)_6][BAR_4F]_2$, *Inorg. Chem.* **2014**, *54*, 352–358.
 11. D. S. Weinberger, M. Melaimi, C. E. Moore, A. L. Rheingold, G. Frenking, **P. Jerabek**, G. Bertrand, Isolation of Neutral Mono- and Dinuclear Gold Complexes of Cyclic (Alkyl)(amino)carbenes, *Angew. Chem. Int. Ed.* **2013**, *52*, 8964–8967.
 10. M. Molon, C. Gemel, R. W. Seidel, **P. Jerabek**, G. Frenking, R. A. Fischer, The Organozinc Rich Compounds $[Cp^*M(ZnR)_5]$ ($M = Fe, Ru$; $R = Cp^*, Me, Cl, Br$), *Inorg. Chem.* **2013**, *52*, 7152–7160.
 9. **P. Jerabek**, G. Frenking, Structures and energies of C_4S_4q ($q = +1, 0, -1$) isomers. A theoretical study, *Int. J. Mass. Spectrom.* **2013**, *354–355*, 342–345.
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