Paul Jerabek

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

Email paul.jerabek@hereon.de **ORCID** 0000-0002-2995-9755 **Scholar** profile
LinkedIn paul-jerabek

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 oganesson; 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**, *Philipps-Universität Marburg* 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**, *Philipps-Universität Marburg* 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 – present	**Hydrogen Technology** Co-lecturer, Technische Universität Hamburg (TUHH), Hamburg

2019 **Knowledge for Tomorrow – Cooperative Research Projects in Sub-Saharan Africa (Volkswagen-Stiftung)**
Tutor, University of Mauritius, Reduit

2014 – 2015 **Lectureship**
Lecturer, Technische Hochschule Mittelhessen, Gießen

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 **Chemiedozenzentagung 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, Ni–Cr Substitution in TiFe: An Integrated Experimental–Modeling Study of Phase Stability and Hydride Thermodynamics, *Adv. Energy Sustain. Res.* **2026**, *7*, e70243.

69. J.-E. Ahrens, **P. Jerabek**, L. Vondung, Relativistic effects are crucial for uranium-phosphorus 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 FeTi by ab initio thermodynamic modelling of Fe–Ti–Si phase equilibria, *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 of metal-hydride interphases—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 and RuII complexes via choice of azine: correlation of ligand pKa with Epa(MIII/II) of complex, *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 valance 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. Ovri, 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. Bondì, 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. Bondì, 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 Reevaluated: 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 Hänisch, 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)(η(6)-toluene) and Ni(I)(η(5)-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 N2 and P2 versus tetrahedral N4 and P4, *Theor. Chem. Acc.* **2014**, *133*, 1447-1456.

13. N. B. Jaufeerally, P. Ramasami, **P. Jerabek**, G. Frenking, Bonding analysis of telluroketones H2A=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 [Zn2]2+ Trapped In A Homoleptic Metalloid Coordination Environment Stabilized by Dispersion Forces: [Zn2(GaCp*)6][BAr4F]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 C4S4q (q=+1, 0, -1) isomers. A theoretical study, *Int. J. Mass. Spectrom.* **2013**, *354-355*, 342–345.

8. M. H. Holthausen, S. K. Surmiak, **P. Jerabek**, G. Frenking, J. J. Weigand, [3+2] Fragmentation of an [RP5Cl]+ Cage Cation Induced by a N-Heterocyclic Carbene, *Angew. Chem. Int. Ed.* **2013**, *52*, 11078–11082.

7. C. Ganesamoorthy, S. Loerke, C. Gemel, **P. Jerabek**, M. Winter, G. Frenking, R. A. Fischer, Reductive elimination: A pathway to low-valent aluminium species, *Chem. Commun.* **2013**, *49*, 2858–2860.

6. S. R. Barua, W. D. Allen, E. Kraka, **P. Jerabek**, R. Sure, G. Frenking, Nearly Degenerate Isomers of C(BH)2 : Cumulene, Carbene, or Carbone?, *Chem. Eur. J.* **2013**, *19*, 15941–15954.

5. A. Yu. Rogachev, **P. Jerabek**, S. Klein, G. Frenking, R. Hoffmann, Hunting dimers, *Theor. Chem. Acc.* **2012**, *131*, 1-11.

4. M. Donath, E. Conrad, **P. Jerabek**, G. Frenking, R. Fröhlich, N. Burford, J. J. Weigand, Ligand-Stabilized [P(4)](2+) Cations, *Angew. Chem. Int. Ed.* **2012**, *51*, 2964–2967.

3. F. Dielmann, O. Back, M. Henry-Ellinger, **P. Jerabek**, G. Frenking, G. Bertrand, A crystalline singlet phosphinonitrene: a nitrogen atom-transfer agent, *Science* **2012**, *337*, 1526-1528.

2. T. Bollermann, M. Molon, C. Gemel, K. Freitag, R. W. Seidel, M. von Hopffgarten, **P. Jerabek**, G. Frenking, R. A. Fischer, Oligonuclear molecular models of intermetallic phases: a case study on [Pd2Zn6Ga2(Cp*)5(CH3)3], *Chem. Eur. J.* **2012**, *18*, 4909–4915.

1. T. Bollermann, K. Freitag, C. Gemel, M. Molon, **P. Jerabek**, G. Frenking, R. A. Fischer, The Rich Chemistry of [Zn2Cp*2]: Trapping Three Different Types of Zinc Ligands in the PdZn7 Complex [Pd(ZnCp*)4(ZnMe)2{Zn(tmeda)}], *Inorg. Chem.* **2011**, *4*, 10486–10492.