GESELLSCHAFT DEUTSCHER CHEMIKER
ORTSVERBAND SIEGEN

Ankündigung

Am Dienstag, **8. November 2022**, spricht um **16:30 Uhr**
im Hörsaal AR-F 002 des Departments Chemie und Biologie

Prof. Dr. Dr. h.c. Martin Jansen

Max-Planck-Institut für Festkörperforschung, Stuttgart

über das Thema

„Pride and Prejudice - Musings about Purposeful Solid State Synthesis“

Kaffeerunde ab 16 Uhr im Foyer des Hörsaals AR-F 002, organisiert durch das JungChemikerForum Siegen

Alle interessierten Kolleginnen und Kollegen, Mitarbeiterinnen und Mitarbeiter und Studierende sind zu diesem Vortrag herzlich eingeladen.
Gäste sind herzlich willkommen.

Der Ortsverbandsvorsitzende
PD Dr. Stephan Bäurle
Tel. 0271 740-4025

GESELLSCHAFT DEUTSCHER CHEMIKER

ORTSVERBAND SIEGEN

Prof. Dr. Dr. h.c. Martin Jansen

Pride and Prejudice - Musings about Purposeful Solid State Synthesis

Relevance, or utility, of results seems to have arrived at the first rank of priorities in chemical sciences. For synthesis, this is meaning that success is rather assessed by performance of a new compound, basically as a drug or a material. Unfortunately, the number of positive hits in this respect compared to the total of newly synthesized compounds is disappointingly low. This fact clearly reflects lack of predictability of properties of compounds, and in the solid state synthesis regime, even of composition and structure. Assuming that the chemists´ playground comprises 86 stable elements, the number of possible combinations, each containing numerous individual stable configurations, is breathtaking:

$$\sum_{n=0}^{86} \binom{86}{n} = 2^{86}$$

The approaches developed in tackling the task of exploring this space in a purposeful fashion have been based on heuristic concepts like building bloc assembly, thermodynamic considerations, or crystal chemical rules. We now seem to have arrived at a turning point in as much as new extended solids without precedent have been predicted computationally and subsequently synthesized.[1] Taking these computational approaches one faces a critical issue: would this enable to spot literally any chemical configuration capable of existence, even if it features unconventional, unprecedented characteristics? Recent observations are nourishing scepticism in this direction. Experimentally discovered compounds that would have escaped current computational prediction are, e.g., crucially stabilized by the (configurational) entropic contribution of localized, however, disordered electrons,[2] p-electron systems that

feature singular structural, electronic and magnetic ordering schemes,[3] or oxides with integer stoichiometry displaying weird compositions and uncommon chemical bonding.[4]
In the lecture, an attempt will be undertaken to shed light on this dichotomy.

References

[1] *M. Jansen,* Synergies and competition between current approaches to materials discovery C. R. Chimie **21** (2018) 958 – 968; *M. Jansen,* Conceptual Inorganic Materials Discovery – A Road Map Adv. Mater. **27** (2015) 3229 – 3242.
[2] *C. Freysoldt, P. Merz, M. Schmidt, S. Mohitkar, C. Felser, J. Neugebauer, M. Jansen:* Discovery of Elusive K_4O_6, a Compound Stabilized by Configurational Entropy of Polarons, Angew. Chem. Int. Ed. **58** (2019) 149 – 153.
[3] *T. Knaflič, P. Jeglič, M. Komelj, A. Zorko, P. K. Biswas, A. N. Ponomaryov, S. A. Zvyagin, M. Reehuis, A. Hoser, M. Geiß, J. Janek, P. Adler, C. Felser, M. Jansen, D.Arčon:* Spin-dimer ground state driven by consecutive charge and orbital ordering transitions in the anionic mixed-valence compound Rb_4O_6, Phys. Rev. B **101** (2020) 024419.
[4] *A. Kovalevskiy, C. Yin, J. Nuss, U. Wedig, M. Jansen,* Uncommon structural and bonding properties in $Ag_{16}B_4O_{10}$ Chem. Sci. **11** (2020) 962-969; *G. S. Thakur, R. Dinnebier, T. C. Hansen, W. Assenmacher, C. Felser, M. Jansen,* Idiosyncratic $Ag_7Pt_2O_7$: An Electron Imprecise yet Diamagnetic Small Band Gap Oxide Angew. Chem. Int. Ed. **59** (2020) 19910 – 19913.