

SEMINARIUM RENTGENOWSKIE

Seminarium w trybie stacjonarnym

Laboratorium SL-1 zaprasza na seminarium, które odbędzie się
dnia **15.04.2025 r.** o godz. **10:30** w **Sali D**

Tytuł Seminarium:

High-pressure chemistry and physics of fluorides

Current diamond anvil cell (DAC) techniques enable performing routine measurements on solids compressed to 100 GPa (million atmospheres). At such conditions the pressure-volume work term (pV) becomes comparable to covalent bond energies therefore considerably affecting the chemistry, structure, and properties of compounds that are otherwise well known and characterized under ambient conditions. [1,2]

Through a combination of Raman spectroscopy and synchrotron powder X-ray diffraction measurements supplemented with density functional theory (DFT) calculations we unraveled the pressure response of two fluoride systems. The first was K_2CuF_4 , a prototypical 2D ferromagnetic system. We found that at 10 GPa sliding of $[\text{CuF}_4]^{2-}_{\infty}$ layers leads to a transition from the Ruddlesden–Popper phase into a Dion–Jacobson-like structure. This transition results in substantial structural and electronic rearrangement within the planes, resulting in a change from 2D ferromagnetism to 1D antiferromagnetism. [3]

The second system is palladium trifluoride which despite its seemingly simple stoichiometry is a mixed-valent system better formulated as $\text{Pd}^{\text{II}}\text{Pd}^{\text{IV}}\text{F}_6$. We performed an attempt to verify whether application of high pressure might force this compound to form a genuine Pd^{III} fluoride ($\text{Pd}^{\text{III}}\text{F}_3$). Indeed, hybrid density functional calculations predict the thermodynamic preference for single-valent (comproportionated) polymorphs at pressures exceeding 30 GPa. Experimentally we found two phase transitions, with the second one, commencing at ~50 GPa, introducing a monoclinic $C2/c$ phase containing genuine Pd^{III} centers. Preliminary data suggests that this phase might host strong one-dimensional antiferromagnetic spin-spin interactions.

References

- [1] W. Grochala, R. Hoffmann, J. Feng, N. W. Ashcroft, *Angew. Chemie Int. Ed.* 46, 3620, 2007.
- [2] L. Zhang, Y. Wang, J. Lv, Y. Ma, *Nat. Rev. Mater.* 2, 17005.

[3] S. B. Pillai, D. Upadhyay, J. Drapała, Z. Mazej, D. Kurzydłowski, *J. Phys. Chem. C* 128, 17747, 2024.

Prelegent: **dr hab. Dominik Kurzydłowski, profesor UKSW**

Afiliacja Prelegenta: **Uniwersytet kardynała S. Wyszyńskiego**

dr hab. Aleksandra Drzewiecka - Antonik

dr hab. inż. Ryszard Sobierajski, prof. IF PAN