1. PHD PROJECT DESCRIPTION (4000 characters max., including the aims and work plan)

Project title: ***Green transition in the area of precursor synthesis and production of micro- and nanomaterials from the gas phase***

1.1. Project goals

- development of finding 'greener' and 'green' new precursors dedicated to specific vapor deposition techniques,
- synthesis using mechanochemistry and limited solvent methods,
- studies of reactions in the gas phase and solid state,
- understanding mechanisms of electron/ion and laser beam interactions with adsorbed molecules,
- selection of promising precursors,
- obtaining micro- and nanomaterials with defined properties,
- applications of fabricated materials in 'green' nanotechnology.

1.2. Outline

Micro and nanomaterials containing transition metals are used in electronics, optoelectronics, plasmonics, catalysis, and antimicrobial agents. They can be obtained by gas-assisted methods such as chemical vapor deposition (CVD), where one or more volatile precursors are transported to the reactor chamber and decompose on a heated substrate. Nowadays, methods for decomposition using other factors are becoming more significant. The advanced process, so-called 3D nano-printing, such as e.g., focused electron beam induced deposition (FEBID) or focused ion beam induced deposition (FIBID), allows obtaining deposits of a unique composition or shape. Therefore, volatile metal complexes, which consist of an 'ink', play a crucial role in the success during the deposition, and they influence the development of nanotechnology.
Currently, the synthesis of precursors is carried out using classical methods with significant solvent consumption. In addition, volatility-enhancing substituents mostly contain fluorinated groups, so-called PFAS compounds, which should be limited or even excluded from use in line with global trends. Therefore, it is necessary to look for complexes with reduced content of this element. However, they should still be able to generate volatile metal carriers at low temperatures, which are transported over a substrate where they decompose, forming the desirable material. New 'greener' and user-friendly precursors, which can be used in the one-step fabrication of materials, are still sought.

The main aim of the proposed project is to find new 'greener' volatile precursors and synthesize them using mechanochemical or solvent-limited methods. Select compounds capable of producing micro- and nanomaterials used in 'green' commercial applications.

1.3. Work plan

- Classic and 'green' synthesis of new potential precursors,
- Complexes' composition and structure studies,
- Determination of volatility and thermal stability of the compounds,
- The use of calculations to find or confirm the relation between molecules' structure and physicochemical properties,
- Studies of molecule sensitivity to electrons or ions, a laser beam, and plasma treatment. Propose mechanisms of interactions for promising precursors,
- Fabrication of nano- and micromaterials for 'green' applications
- Morphology, composition, and properties characteristics of the obtained materials,
- Studies of the activity of promising selected materials.

1.4. Literature *(max. 7 listed, as a suggestion for a PhD candidate preliminary study)*

1) I. Utke, P. Swiderek, K. Höflich, K. Madajska, J. Jurczyk, P. Martinović, I. B. Szymańska, *Coordination Chemistry Reviews,* 458 (2022) 213851.
2) S. Barth, M. Huth, F. Jungwirth *J. Mater. Chem. C 2020, 8*, 15884-15919.
3) P. Martinović, M. Rohdenburg, A. Butrymowicz, S. Sarigül, P. Huth, R. Denecke, I. B. Szymańska, P. Swiderek, *Nanomaterials,* 12 (2022) 1687.
4) Javier F. Reynes, Felix Leon, Felipe García, *ACS Org. Inorg. Au Au,* (2024), 4, 432−470.
5) L. Berger, K. Madajska, I. B. Szymańska, K. Höflich, M. N. Polyakov, J. Jurczyk, C. Guerra-Nuñez, I. Utke, *Beilstein J. Nanotechno*l, 9 (2018) 224–232.
6) R. Córdoba, P. Orús, S. Strohauer, T. Torres, J. M. De Teresa, *Scientific Reports*, 9 (2019) 14076.
7) Butrymowicz-Kubiak Aleksandra, Muzioł Tadeusz, Kaczmarek-Kędziera Anna, Jureddy Chinmai S., Maćkosz Krzysztof, Utke Ivo, Szymańska Iwona B., *Dalton Transactions*, 53 (2024), 13662-13677, DOI:10.1039/d4dt01287a.

1.5. Required initial knowledge and skills of the PhD candidate

- Analytical thinking
- Eager to learn
- Teamwork

- Experience in basic chemical synthesis and spectroscopy
- Understanding of nano- and micromaterials synthesis and analysis
- Basic knowledge of deposition techniques and 'green transition'
- Keen to learn new techniques, instrumentations, and calculations
- Thinking oriented on innovation and application

1.6. Expected development of the PhD candidate's knowledge and skills

- Improve analytical thinking,
- Understanding why we still need to learn,
- Organization of teamwork,
- High experience in advanced chemical synthesis, including mechanochemistry,
- Extensive experience in spectroscopic data analysis,
- Fluency in materials synthesis and analysis,
- Advanced knowledge of deposition techniques,
- Knowledge of modern techniques and instrumentation, and the ability to do calculations,
- Thinking highly focused on innovation, application, and the introduction of 'green chemistry' solutions to studies.