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

Project title: The search for precursors dedicated to specific vapor deposition methods

1.1 Project goals

- development of finding and synthesis of precursors dedicated to specific vapor deposition techniques,
- the use of computational methods to determine the properties of molecules,
- studies of reactions in the gas phase using electron impact mass spectrometry and temperature-variable IR spectroscopy,
- understanding mechanisms of electron and ion beam interactions with thin films of compounds,
- selection of precursors promising for individual vapor deposition methods,
- obtaining 2D and 3D micro- and nanodeposits with defined shapes and compositions.

1.2 Outline

Micro- and nano-structures of transition metals or containing them are used in electronics, optoelectronics, plasmonics, catalysis, and antibacterial and antiviral agents. These structures can be obtained by gas-assisted methods such as chemical vapour deposition (CVD). This is a process where one or more volatile precursors are transported in the vapour carrier gas to the reactor chamber, where they decompose on a heated substrate and deposit a solid material. Nowadays, methods, where decomposition is initiated using other than temperature factors, are becoming more important. The advanced process such as e.g., focused electron beam induced deposition (FEBID), focused ion beam induced deposition (FIBID), plasma enhanced CVD, or laser-assisted CVD allow obtaining deposits of a unique composition or shape. Volatile complexes constitute a topic of intensive studies because they play a crucial role in success during the deposition, and they influence on the development of nanotechnology.

With Vapor Deposition Methods, thin layers of metals and other materials and more complicated 2D and 3D nanostructures can be deposited on different substrates. However, these methods require applying compounds, which are metal sources (so-called precursors). This role is generally played by organometallic or coordination compounds. They have the ability to generate volatile metal carriers, which are transported over a substrate where they decompose, forming the desirable material. New precursors, which easily generate metal carriers, demonstrate low evaporation temperature and can be used in the one-step fabrication of materials, are still sought.

Materials formation can be induced by heating (CVD) but also using a focus electron (FEBID) or ion (FIBID) beam, a laser beam (LACVD), or plasma. The main aim of the proposed project is to find new volatile precursors or to test known and fast fitting them to the mentioned methods. The using of computational methods to find the crucial properties of precursor molecules seems needed. Next deposits are obtained and finally, selected micro- and nanomaterials are studied.

Their conductivity; optical properties; and antibacterial and antiviral activity can be used for commercial applications.

1.3 Work plan

- Synthesis of potential precursors and the composition and structure studies for new complexes,
- The use of computational methods to find the crucial properties of molecules,
- Determination of volatility and thermal stability of the compounds,
- Chemical Vapor Deposition experiments for selected complexes,
- Studies of molecule sensitivity to electrons or ions, a laser beam, and plasma treatment. Propose mechanisms of interactions for promising precursors,
- FEBID and FIBID, laser- and plasma-assisted experiments for selected compounds.

1.4. Literature (max. 10 listed, as a suggestion for a PhD candidate)

1) I. Utke, P. Swiderek, K. Höflich, K. Madajska, J. Jurczyk, P. Martinović, I. B. Szymańska, *Coordination Chemistry Reviews,* 458 (2022) 213851.
2) K. Madajska, I. B. Szymańska, *Materials*, 14 (2021) 3145.
3) S. Barth, M. Huth, F. Jungwirth *J. Mater. Chem. C 2020, 8*, 15884-15919.
4) I. Utke, S. Moshkalev, P. Russell, *Nanofabrication Using Focused Ion and Electron Beams: Principles and Applicatio*ns, Oxford University Press. 2011, 3; 11-14.
5) M. Lacko, P. Papp, I. B. Szymańska, E. Szłyk, S.Matejcik, *Beilstein J. Nanotechnol.*, 9 (2018) 384–398.
6) 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.
7) K. Höflich, J. M. Jurczyk, K. Madajska, M. Götz, L. Berger, C. Guerra-Nuñez, C. Haverkamp, I. Szymańska, I. Utke, *Beilstein J. Nanotechnol*, 9 (2018) 842–849.
8) L. Sala, I. B. Szymańska, C. Dablemont, A. Lafosse, L. Amiaud, *Beilstein J. Nanotechnol.*, 9 (2018) 57–65.
9) P. Martinović, M. Rohdenburg, A. Butrymowicz, S. Sarigül, P. Huth, R. Denecke, **I. B. Szymańska**, P. Swiderek, *Nanomaterials,* 12 (2022) 1687
10) R. Córdoba, P. Orús, S. Strohauer, T. Torres, J. M. De Teresa, *Scientific Reports*, 9 (2019) 14076.

1.5 . Required initial knowledge and skills of the PhD candidate

- Analytical thinking
- Eager to learn
- Teamwork
- Experience in chemical synthesis and spectroscopy
- Understanding of materials synthesis and analysis
- Basic knowledge of deposition techniques
- 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 chemical synthesis and spectroscopy,
- Fluency in materials synthesis and analysis,
- Advanced knowledge of deposition techniques,
- Knowledge of modern techniques and instrumentation and ability to do calculations,
- Thinking highly oriented on innovation and application.