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We have been appreciating noble metals for over 6000 years. Color, shines, high density, malleability, high stability, resistant to corrosion and oxidation, timelessness – this asset was decisive for the range of applications of noble metals (ruthenium, rhodium, palladium, silver, osmium, iridium, platinum, and gold). Thanks to the outstanding resistance even to an aggressive chemical environment and high temperature, high electrical and thermal conductivity, catalytic properties, these metals are also invaluable for nanotechnology. Noble metals found application in integrated circuits: as electrodes in dynamic random access memories (DRAMs), as gates in transistors, as seed and barrier layers for copper in interconnect metallization in microchips, as well as in catalysis, sensors, and magnetic data storage. Nanometer-thin films of noble metals are therefore of high importance in current and future technologies.

The super-thin structure of the material can be obtained by atomic layer deposition (ALD) technique, which provides perfect coatings even of complex three-dimensional structures. This technique is based on the principle of sequential chemical reactions of reactants on a solid substrate, as a result the material is deposited the atomic layer by the atomic layer. Therefore, the deposition of noble metals thin layers, which by definition are chemically inert, is a challenge.

The major challenge in metal ALD is the reduction process to yield the metallic target film from metal source, that usually comprise of metal cation surrounded by anionic ligands. Existing strategies involve using reducing agent or, counterintuitively, oxidizing agent as second co-reagent. Using reducer as co-reagent, *e.g.* H_2-plasma, can lead to an abbreviated cycle, and reduced rate of deposition, when stable surface intermediates are not available. In process using oxidizing agent, *e.g.* O_2-plasma, the reduction of metallic center is a result of precursor decomposition at the catalytic surface, with the danger of surface poisoning and oxide deposition. In both scenarios, nature of surface species determines ALD success.

The aim of the research project is the computational design of chemical processes, that facilitate atomic layer deposition of nanometer-thin layers of noble metals. Computational modelling offers complementary analysis by providing a much greater insight into the reaction mechanisms, specifically by revealing intermediate steps that are not easily observed experimentally. The mechanisms of the formation of noble metal nuclei and the individual stages of the layer deposition sequence will be investigated. Factors that facilitate nucleation will be identified. Furthermore, some speculations regarding formation of certain by-products, transient surface structures and intermediates products will be cleared out. This will allow to propose appropriate reagents and chemical processes to control and improve efficiency of the atomic layer deposition of noble metals. This will pave way for commercial applications.