



Contribution ID : 11

Type : **Oral Presentation**

New aspects of U(V) chemistry in oxo-materials: from ambient to extreme conditions

Wednesday, 1 November 2017 16:15 (30)

Using extreme pressure (10GPa/1200°C) we obtained a new modification of U₂O₅ with an extraordinary dense structure. The crystal structure of resulting HP (high pressure)-U₂O₅ is dramatically differs from ambient pressure polymorph so called delta-U₂O₅. The structure of HP-U₂O₅ is more related to the cubic UO₂ than to the layered delta-U₂O₅. Using state of the art ab initio methods we reveal the stability ranges of both ambient and high pressure forms of U₂O₅ and demonstrated a potential pathway of phase transition under pressure. In second case we demonstrated that the pentavalent uranium (U(V)) can be stabilized in [Ln(UVO₂)W₄O₁₄] (Ln = Nd-Tm and Y) series via aliovalent substitution of Ca²⁺ cations. We confirmed U(V) stabilization using state of the art methods such as U M4 edge high energy resolution X-ray absorption near edge structure (HR-XANES).Magnetic study reveals low temperature ordering of 5f₁ and 4f_n systems. All the phases tend to demonstrate the antiferromagnetic properties with significant difference between pure 5f₁ system (Y-beating phase) and 5f₁-4f_n compounds (Nd-Tm).

Summary

Primary author(s) : Prof. ALEKSEEV, Evgeny (Forschungszentrum Jülich)

Presenter(s) : Prof. ALEKSEEV, Evgeny (Forschungszentrum Jülich)

Session Classification : Ceramic and Glass-Ceramic Wasteforms

Track Classification : National and international collaborative waste management programs