Session of Focus Materialchemie – Wednesday, **18.01.2022** 16:00 – @ Seminarraum Lehar 02 (TU-Wien, Getreidemarkt 9, BC, OG. 02, room A46) – join us on ZOOM (ID: 983 0066 2349)

Structural and energetic description of transition metal compounds with advanced density functionals

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A correct energetic description is a fundamental parameter to reach chemical accuracy with computational methods. The ground state energy, for example, determines the stability of crystal structures for polymorphic compounds, and the formation energy indicates the overall chemical stability. The fundamental methods to computationally obtain such parameters are under continuous development. While main group compounds are generally easier to describe with density functional theory (DFT), the method of choice in this work, the main emphasis here is on transition metal compounds which feature correlated electrons. For this, two state-of-the-art functionals, PBE and SCAN, are enhanced with the on-site hybrid functional EECE and compared to each other regarding the polymorphic energy ordering and formation energy. The results for the polymorphic energy ordering show a benefit for both pairings with the EECE functional, where SCAN-EECE gives the best predictions. However, the calculation of the formation energy offers mixed results. SCAN tends to underestimate the formation energy, whereas SCAN-EECE overestimates it.