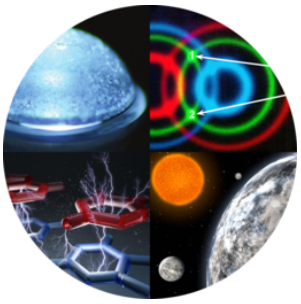

Münchner Physik-Kolloquium

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Dieses Semester findet das Kolloquium online statt: https://tum-conf.zoom.us/j/93234766313

Festkolloquium für Professor Winfried Petry

Ab initio descriptors to guide materials design in high-dimensional chemical and structural configuration spaces

Prof. Dr. Jörg Neugebauer, *Max-Planck-Institut für Eisenforschung, Düsseldorf*

Monday, 21 June 2021, 17:15 h
https://tum-conf.zoom.us/j/93234766313 Meeting-ID: 932 3476 6313 Password: Kolloquium
Please install the software in advance.

Modern engineering materials have evolved from simple single phase materials to nano-composites that employ dynamic mechanisms down to the atomistic scale. The structural and thermodynamic complexity of this new generation of structural materials presents a challenge to their design since experimental trial-and-error approaches as successfully used in the past are often no longer feasible. Ab initio approaches provide perfect tools to new design routes but face serious challenges when having to systematically sample high-dimensional chemical and structural configuration spaces. Combining advanced sampling approaches with our python based framework *pyiron* allows us in a highly automated way to combine first principles calculations with big data analytics and to obtain accurate ab initio descriptors. The flexibility and the power of these approaches will be demonstrated for a few examples: The design of ductile Mg alloys, overcoming mutually exclusive properties in high entropy alloys, and the discovery of general rules for interstitials in metals.