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QUANTUM MECHANICALLY GUIDED MATERIALS DESIGN FOR SURFACE ENGINEERING

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The combination of modern electronic structure calculations with the highly efficient combinatorial thin film composition-spread method constitutes an effective tool for knowledge based materials design of hard and wear resistant coatings as well as of thin film metallic glasses. Besides elastic properties and phase stability also the interaction of the coating with the ambient can be described based on quantum mechanics. In the talk predictions of the interaction of coated tool surfaces with gases contained in the atmosphere as well as materials to be formed are discussed. Transition metal nitride and oxynitride as well as boride coatings used for forming operations of Al and Polymers are investigated and experimental data characterizing these interactions will be discussed. Furthermore, the implications of the presence of point defect for the thermal stability of TiAlN [1] will be analyzed and hybridization implications for the damage tolerance of thin film metallic glasses will be presented [2].

References

[1] M. to Baben et al., Materials Research Letters (2016)

[2] V. Schnabel et al., Scientific Reports (2016)

SHORT BIO

Jochen M. Schneider, Ph.D., is Professor of Materials Chemistry at RWTH Aachen University, Germany. Formerly at Linköping University, Sweden, and Northwestern University, USA, Jochen received his Ph.D. degree in surface engineering from Hull University, UK. His research interest is the materials science of thin films grown by plasma-assisted vapour deposition. In Aachen his research focus was quantum-mechanically guided design of thin films regarding elasticity and phase stability.

Jochen has been awarded the Sofya Kovalevskaya Prize by the Alexander von Humboldt and was named a Fellow of AVS in 2013 and Max Planck Fellow as well as RWTH Fellow in 2015.