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## Quantum mechanically guided materials design for surface engineering

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The combinatorial approach, combining combinatorial materials synthesis of thin film composition-spreads with high-throughput property characterization has proven to be a powerful tool to delineate composition-structure-property relationships, and hence to efficiently identify composition windows with enhanced properties. [1] 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. [2-4] Besides the elastic property 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 [5-7] contained in the atmosphere as well as materials to be formed are discussed. Coatings used for forming operations of Al [8] and Polymers [9] are investigated and initial experimental data characterizing these interactions will be discussed.

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