

**MATERIALWISSENSCHAFTLICHES KOLLOQUIUM**

**am 27.07.2011**

um 17.15 Uhr – Raum 1520, Geb. K, DE 15

**First-principles modeling of mechanical properties: simple models  
and hard numbers**

**Prof. Dr. Raimund Podloucky**

*Universität Wien*

Density functional theory is applied for calculating cleavage, elastic and related properties. The aim is to provide hard numbers derived from simple models which might assist the materials scientist in the search for hard and resistible materials.