

Statistical Mechanics from First Principles

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This talk sketches the methods and describes recent theoretical work performed with *ab initio* atomistic thermodynamics and *ab initio* statistical mechanics (molecular dynamics as well as kinetic Monte Carlo).

Key examples in this talk concern the puzzle of O₂ dissociation at Al(111), in particular emphasizing the role of the O₂ spin state, and the properties of transition metals in oxygen atmospheres with (T, p) settings ranging from UHV to those encountered at “human” (or higher T, p) conditions.

Analyzing oxidation catalysis at the late transition metals it is found that the surface composition, that is attained under reactive conditions, and the consequential functionality of the surface can be very different from what is found at (or close to) thermodynamic equilibrium.