RCMS Research Center for Materials Science

IGER Nagoya University

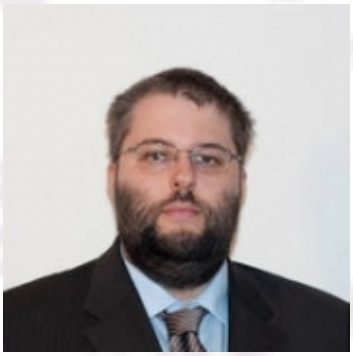
Nagoya University

Theoretical Chemistry Colloquium

September 3, 2013 (Tue), 16:00-17:00

Chemistry Gallery, RCMS 2nd floor

Advanced Modeling of Functional Nanoionics in Oxides



Dr. Jan M. Knaup
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Abstract: *Oxide materials exhibit a variety of interesting properties for emerging technologies, including solar energy, biofuel production and beyond-CMOS logic. In all these applications, the nanoscale dynamics of ions and vacancies are highly important. One particulary interesting example is the memristive effect in slightly reduced metal oxides, such as TiO_{2-x}, which is governed by the migration and accumulation of oxygen vacancy defects and resulting phase transformations into Magnéli phases of Ti_nO_{2n-1} composition. The vacancy is no physical object by itself but an emergent property of the defective crystal, and its hops between lattice positions are rare events. Therefore a combination of advanced structural analysis techniques and rare event simulation methods is necessary to understand the dynamics of this system.*

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