Saulėtekio Puslaidininkių Fizikos Seminaras

CENTER FOR PHYSICAL SCIENCES AND TECHNOLOGY

VILNIAUS UNIVERSITETAS · 1579 · FIZIKOS FAKULTETAS

J. Christian Schön
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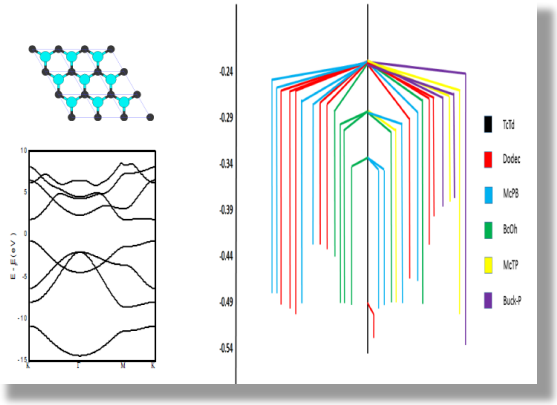
Complex energy landscapes and their applications in chemistry, physics, and nanomaterials

2018-06-05 16:00 / NFTMC D401, Saulėtekio 3



In many areas of science, problems are frequently encountered which exhibit an underlying complex multi-minima energy landscape. To address these questions and deal with the time evolution of such systems, it is necessary to develop new general concepts. In this talk, I am going to give an introduction to basic landscape concepts such a local ergodicity and generalized barriers, together with presenting algorithms that go beyond standard global optimization techniques. These are illustrated by a number of examples, including crystals, molecules, clusters, or amorphous ceramics.

coffee & snacks by BROLIS SEMICONDUCTORS & Young Minds

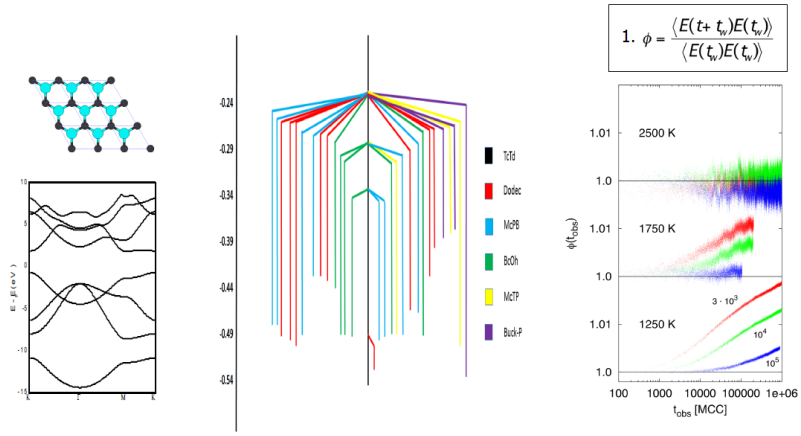
Title: Complex energy landscapes and their applications in chemistry, physics, and nanomaterials

Speaker: (Prof. Dr.) J. Christian Schön, MPI for Solid State Research, Stuttgart, Germany

Abstract: In many areas of science, problems are frequently encountered which exhibit an underlying complex multi-minima energy landscape. Examples range from aging in physical and chemical systems to metastable chemical compounds and glassy systems, and optimal control of e.g. crystal growth, just to name a few instances. To address these questions and deal with the time evolution of such systems, it is necessary to develop new general concepts for analyzing such landscapes and suitable global exploration algorithms to obtain global and local information about the structure of the energy landscape.

In this talk, I am going to give an introduction to basic landscape concepts such a local ergodicity[1,2,3] and generalized barriers[4,2], together with presenting algorithms that go beyond standard global optimization techniques[2]. These are illustrated by a number of examples, including the structure prediction via global exploration of energy landscapes of chemical systems such as crystals[3], molecules[2], clusters[5], or monolayers[6], applications of optimal control in chemical synthesis[7], and aging in amorphous ceramics[8].

[1] J. C. Schön: *Structure Prediction and Modelling of Solids: An Energy Landscape Point of View* (Proceedings of the RIGI workshop on Predictability of physical properties of crystals (Luzern, Switzerland, Mai 1998)
[2] J. C. Schön, C. Oligschleger, J. Cortes: *The threshold algorithm: Description of the methodology and new developments*, Journal of Chemical Physics, (2017), **147**, 152713
[3] J. C. Schön: *Nanomaterials - What energy landscapes can tell us*, Processing and Applications of Ceramics, (2015), **9**, 157-168
[4] J. C. Schön, M.A.C. Wevers, M. Jansen: *Entropically stabilized region on the energy landscape of an ionic solid*, Journal of Physics: Condensed Matter, (2003), **15**, 5479-5486
[5] C. J. Heard, R. L. Johnston, J. C. Schön: *Energy landscape exploration of sub-nanometre copper-silver clusters*, ChemPhysChem, (2015), **16**, 1461-1469
[6] R. Gutzler, J. C. Schön: *Two-dimensional Silicon-Carbon Compounds: Structure Prediction and Band Structures*, Zeitschrift für Anorganische und Allgemeine Chemie, (2017), **643**, 1368-1373
[7] J. C. Schön: *Finite-Time Thermodynamics and the Optimal Control of Chemical Syntheses*, Zeitschrift für Anorganische und Allgemeine Chemie, (2009), **635**, 1794-1806
[8] A. Hannemann, J. C. Schön, M. Jansen, P. Sibani: *Nonequilibrium Dynamics in Amorphous $Si_3B_3N_7$*, Journal of Physical Chemistry B, (2005), **109**, 11770 - 11776


-0.24
-0.29
-0.34
-0.39
-0.44
-0.49
-0.54
TcTd
Dodec
McP6
BcOh
McTP
Buck-P
1. $\phi = \frac{\langle E(t+t_w)E(t_w)\rangle}{\langle E(t_w)E(t_w)\rangle}$
2500 K
1750 K
1250 K
$3 \cdot 10^3$
10^4
10^5
1.01
1.0
$\phi(t_{obs})$
100
1000
10000
100000
1e+06
t_{obs} [MCC]