

RbBi4 (5 ES)

Insight from Band Structures Or : ,How to digest Spaghetti'

A one-day workshop

July 27th, 2018

Max Planck Institute for Solid State Research, Stuttgart

Band structures describe the dispersion of singleelectron energies in reciprocal space and their calculation provides an "ab-initio" method to investigate the electronic structure in crystalline solids. However, the relation of the band structure to concepts, such as the existence of quasiparticles or the notion of chemical bonds,

can be challenging. This workshop shows how to untangle the band structure and thus access a physical understanding of solids. Furthermore, new developments in band structure theory will be presented.

Max Planck Institute for Solid State Research, Stuttgart, Germany

Theoretical Chemistry Group, University of Torino, Italy

Speaker

Institute of Materials Chemistry, TU Wien, Austria

Topic

Juri Grin Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Beate Paulus

Peter Blaha

Nikolay Bogdanov

Roberto Dovesi

Physical and Theoretical Chemistry, Freie Universität Berlin, Germany

Andreas Rost

School of Physics & Astronomy, University of St. Andrews, Scotland, UK

Andreas Savin UPMC Sorbonne Universités, Paris, France

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More Information http://www.fkf.mpg.de/BS2018

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lexander von Humboldt

Program Schedule

Werner-Köster Lecture Hall (2R4) Max Planck Institute for Intelligent Systems Heisenbergstraße 3 • 70569 Stuttgart, Germany

8:30	Registration	
8:50	Welcome	
9:00	Andreas Savin	Do benchmar of density fun
9:40	Roberto Dovesi	Quantum med in semicondue
10:20	Coffee Break	
10:40	Peter Blaha	Calculations o insulating and
11:20	Beate Paulus	Tuning band g
12:00	Lunch	
13:20	Poster Session	
14:20	Andreas Rost	Charge carrier electron syste
15:00	Nikolay Bogdanov	Many-body all correlated ele
15:40	Coffee Break	
16:00	Juri Grin	Normal physic
16:40	Hidenori Takagi	What do I war quantum cher
17:20	Ulrich Wedig	Numbers and
18:15	Barbecue	
20:00	Round Table Discussion	



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chanical treatment of defects ctors: Something new?

f NMR parameters in metallic solids.

gaps in multilayer compounds.

rs in strongly correlated ms - insights from DFT.

initio methods for ctrons in solids.

ology of Spaghetti nutrition.

nt to learn from mistry of oxides?

Images.