

Core-to-core Japan-Germany Workshop, Forschungszentrum Jülich, Nov. 5th-6th 2013

Tuesday, Nov. 5th 2013

9:00-9:05	Welcome Address	
9:05-9:40	K. Sato	Computational design of solar cell materials
9:40-10:15	T. Schena	Iron pyrite in bulk and surface phase: implication on photovoltaic performance
10:15-10:50	R.A. Eichel	Atomic-scale processes during electrochemical energy storage – current understanding and open questions
10:50-11:20	Coffee break	
11:20-11:55	R. Kovacik	Computational Design of Spincalonic Nanostructures
11:55-12:30	H. Ebert	Theoretical description of the anomalous and spin Hall effects in disordered alloys using the Coherent Potential Approximation
12:30-14:00	Lunch	
14:00-14:35	G. Mussler	Molecular-beam epitaxy of topological insulator thin films
14:35-15:10	I. Aguilera	Relativistic GW Calculations for Topological Insulators
15:10-15:40	Coffee break	
15:40-16:15	T. Fukushima	Hubbard U Calculations in Dilute Magnetic Semiconductors
16:15-16:50	P. Mavropoulos	Anisotropy of Spin-Relaxation in Metals
16:50-17:25	S. Doi	Electronic structure calculation of permanent magnets using the KKR Green's function method

19:00 Dinner in Jülich

Wednesday, Nov. 6th 2013

9:00-9:35	H. Kizaki	Ab-initio Study on the Self-regenerating Mechanism of LaFe _{1-x} Pd _x O ₃ Catalyst
9:35-10:10	H. Momida	First-principles study of resistance switching by oxygen vacancies in Al ₂ O ₃ ReRAM
10:10-10:40	Coffee break	
10:40-11:15	R. Mazzarello	Ab initio molecular dynamics simulations of phase-change materials
11:15-11:50	H. Katayama-Yoshida	General Rule of Negative Effective U _{eff} System & Materials Design of High-T _c Superconductors by ab initio Calculations
11:50	Conclusion and Outlook	