cecam Centre Européen de Calcul Atomique et Moléculaire 2018

Reliable and quantitative prediction of defect properties in Ga-based semiconductors

Bremen Center for BCCMS Computational Materials Science

Tuesday, October 09th 2018
(House of Science Bremen/Downtown)

08:00 - 08:50	**Registration**	
08:50 - 09:00	**Opening and welcome, Thomas Frauenheim**	
Session:	**Theory of defects I+II**	***Chair: Peter Deák***
09:00 - 09:40	Alfredo Pasquarello, Swiss Federal Institute of Technology, Lausanne, (Switzerland)	*Limitation to p doping in GaN due to self-compensation*
09:40 - 10:20	Chris G. Van de Walle, University of California, Santa Barbara (USA)	*First-principles studies of of transport and optical properties in sesquioxides*
10:20 - 10:50	**Coffee Break**	
10:50 - 11:30	Su-Huai Wei, Beijing Computational Science Research Center, (China)	*Band structure engineering and doping control of transparent conducting oxides*
11:30 - 12:10	Shengbai Zhang, Rensselaer Polytechnic Institute, Troy, New York, (USA)	*A time-dependent density functional theory molecular-dynamics prediction of non-radiative recombination at the DX center of GaAs:Si*
12:10	**Group photo**	
12:15 - 14:00	**Lunch Break (Restaurant Q1) and Coffee**	
Session:	**Growth and characterization**	***Chair: Klaus Irmscher***
14:00 - 14:40	Martin Eickhoff, University of Bremen (Germany)	*MBE growth of metastable gallium oxide polymorphs*
14:40 - 15:20	Jonathon P. Cottom, University College London (UK)	*The effect of amorphisation on the electronic structure of oxides*
15:20 - 15:50	**Coffee Break**	
	Chair: Michael J. Stavola	
15:50 - 16:30	Manfred Martin, RWTH Aachen University (Germany)	*Gallium oxide-from defects in beta-Ga_2O_3 to amorphous, highly nonstoichiometric a-GaO_x*
16:30 - 17:10	Johan Lauwaert, Ghent University, (Belgium)	*Discriminating defects and device responses in capacitance spectroscopic methods*
19:00 - 21:30	**Welcome Reception (Bremen Town Hall)**	

Wednesday, October 10th 2018
(House of Science Bremen/Downtown)

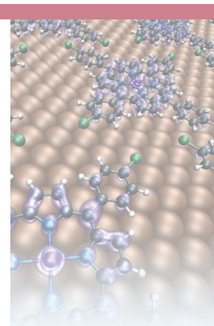
Session:	**Gallium-nitrides, -oxides and -sulfides I**	***Chair: Chris G. Van der Walle***
09:00 - 09:40	Oliver Bierwagen, Paul Drude Institute, Berlin (Germany)	*The transition of defect-related unintentional conductivity from In_2O_3 towards Ga_2O_3*
09:40 - 10:20	Hans Jurgen von Bardeleben, Sorbonne University, Paris (France)	*Gallium vacancy defects in β-Ga_2O_3: a combined electron paramagnetic resonance and theory study*
10:20 - 10:50	**Coffee Break**	
	Chair: Joel B.Varley	
10:50 - 11:30	Walter R. L. Lambrecht, Case Western Reserve University, Cleveland, Ohio (USA)	*Defects in $ZnGeN_2$, an analog of GaN: the dominance of cation antisites*
11:30 - 12:10	Christopher A. Sutton, Fritz Haber Institute of the Max Planck Society, Berlin, (Germany)	*New stable oxides*
12:10 - 14:00	**Lunch Break (Restaurant Q1) and Coffee**	
	CIGS I+II	
Sesson:		***Chair: Suhuai Wei***
14:00 - 14:40	Malgorzata Igalson, Warsaw University of Technology (Poland)	*Photocurrent and capacitance spectroscopy for defect characterization in CIGS*
14:40 - 15:20	Susanne Siebentritt, University of Luxembourg, Belvaux (Luxembourg)	*Defects in $CuGaSe_2$ and $CuInSe_2$: experiment versus theory*
15:20 - 15:50	**Coffee Break**	
	Chair: Stefan Lany	
15:50 - 16:30	Zhi Zeng, Institute of Solid State Physics, Chinese Academy of Sciences, Hefei (China)	*Defect level to intermediate band in Ga-based semiconductor*
16:30 - 17:10	Hannu-Pekka Komsa, Aalto University, Espoo, (Finland)	*Light vs heavy alkali metal impurities in CIGS solar cells*
17:10 - 17:50	Emilio Nogales Díaz, Complutense University of Madrid (Spain)	*Cr as emitting dopant in β-Ga_2O_3 for widely tunable optical mirocavities*
18:40	**Bus Pickup to Conference Dinner**	(Pickup Venue: Radisson Blue Hotel Bremen, Wachtstraße)
19:00 - 22:30	**Conference Dinner (Juergenshof)**	

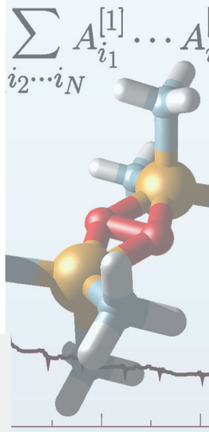
Thursday, October 11th 2018
(House of Science Bremen/Downtown)

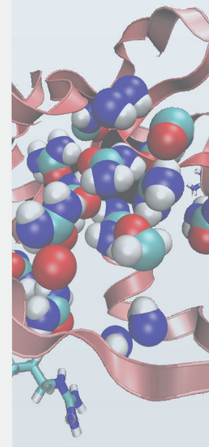
Session:	**Gallium-nitrides, -oxides and -sulfides II**	***Chair: Zhengbai Zhang***
09:00 - 09:40	Klaus Irmscher, Leibniz Institute for Crystal Growth, Berlin (Germany)	*Doping and defects in β-Ga_2O_3*
09:40 - 10:20	Michael J. Stavola, Lehigh University, Bethlehem, Pennsylvania (USA)	*Structure and vibrational properties of OH-centers in beta-Ga_2O_3*
10:20 - 10:50	**Coffee Break**	
10:50 - 11:30	Joel B. Varley, Lawrence Livermore National Laboratory, California (USA)	*Defects and charge localization in Ga-oxides and sulfides*
11:30 - 12:10	Peter Deák, University of Bremen, (Germany)	*Intrinsic carrier trapping and luminescence in beta-Ga_2O_3*
12:10 - 13:30	**Lunch Break (Restaurant Q1) and Coffee**	
Session:	**CIGS II**	***Chair: Susanne Siebentritt***
13:30 - 14:10	Martin Feneberg, Otto von Guericke University, Magdeburg (Germany)	*Influence of many-body effects on optical properties of III-Nitrides*
14:10 - 14:50	Susan Schorr, Helmholtz Center for Materials and Energy, Berlin (Germany)	*A structural perception of intrinsic point defects in CIGS*
14:50 - 15:30	Darius Kuciauskas, National Renewable Energy Laboratory, Golden, Colorado (USA)	*Optical metastability in $CuInGa(Se)_2$ solar cells*
15:30 - 16:10	Christoph Lienau, University of Oldenburg (Germany)	*Coherent manipulation of single and dipole-coupled quantum dots in GaAs-based nanostructures*
17:25	**Poster Mounting**	
17:30 - 21:00	**Poster Session and Catering Buffet**	

Friday, October 12th 2018
(House of Science Bremen/Downtown)

Session:	**Phases and extended defects**	***Chair: Thomas Frauenheim***
09:00 - 09:40	Stephan Lany, National Renewable Energy Laboratory, Golden, Colorado (USA)	*Defect phase diagrams for wide gap and photovoltaic semiconductors*
09:40 - 10:20	Dirk Lamoen, University of Antwerpen, Antwerp (Belgium)	*Structure and electronic properties of defects at grain boundaries in CIGS*
10:20 - 10:50	**Coffee Break**	
10:50 - 11:30	Karsten Albe, Technical University of Darmstadt (Germany)	*First-principles calculations on dislocation-point defect interactions in $Cu(In,Ga)Se_2$ solar cells absorbers*
11:30 - 12:10	Michael Lorke, University of Bremen (Germany	*Carbon in GaN revisted*
12:10 - 12:20	**Closing remarks: Thomas Frauenheim**	







Conference Organisers

Thomas Frauenheim — University of Bremen, Germany; BCCMS; http://www.bccms.uni-bremen.de/cms/people/t-frauenheim/

Peter Deák — University of Bremen, Germany; BCCMS; http://www.bccms.uni-bremen.de/cms/people/p-deak/

Klaus Irmscher — Leibniz Institute for Crystal Growth/ IKZ, Berlin Adlershof, Germany; https://www.ikz-berlin.de/en/research1/simulation-charakterisation/physical-characterization

Susanne Siebentritt — University of Luxembourg; Laboratory for Photovoltaics; http://staff.uni.lu/susanne.siebentritt

Joel B. Varley — Lawrence Livermore National Laboratory, California, US; Center for Interface Science and Catalysis; https://qsg.llnl.gov/jvarley.html

http://www.bccms.uni-bremen.de/veranstaltungen/2018/cecam-ccdyn/

Universität Bremen

Deutsche Forschungsgemeinschaft DFG

cecam Centre Européen de Calcul Atomique et Moléculaire