

Program of the International CECAM-Workshop

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

Bremen Center for Computational Materials Science – BCCMS
University of Bremen, October 8th - 12th 2018
Conference site: House of Science, Downtown

Monday, October 8th 2018 (Radisson Blu Hotel)

18:00 – 21:00 Registration

Tuesday, October 9th 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 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 Irmischer

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-Ga₂O₃ to amorphous, highly non-stoichiometric α -GaO_x

16:30 – 17:10 Johan Lauwaert, Ghent University, Belgium

Discriminating defects and device responses in capacitance spectroscopic methods

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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 de 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

Session:

CIGS I + II

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 microcavities

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- 18:40 **Bus Pickup to Conference Dinner**
(Venue: Radisson Blu Hotel, Wachtstraße)
- 19:00 – 22:30 **Conference Dinner (Restaurant 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 -Ga₂O₃
- 09:40 – 10:20 Michael J. Stavola, Lehigh University, Bethlehem, Pennsylvania, USA
Structure and vibrational properties of OH-centers in beta-Ga₂O₃
- 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-Ga₂O₃
- 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 nanostructure
- 17:25 **Poster Mounting**
- 17:30 – 21:00 **Poster Session, Catering Buffet (House of Science)**

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

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Session:	Phases and extended defects
	<i>Chair: Thomas Frauenheim</i>
09:00 – 09:40	Stephan Lany, National Renewable Energy Laboratory, Golden, Colorado, USA <i>Defect phase diagrams for wide gap and photovoltaic semiconductors</i>
09:40 – 10:20	Dirk Lamoen, University of Antwerp, Antwerp, Belgium <i>Structure and electronic properties of defects at grain boundaries in CIGS</i>
10:20 – 10:50	Coffee Break
10:50 – 11:30	Karsten Albe, Technical University of Darmstadt, Germany <i>First-principles calculations on dislocation- point defect interactions in Cu(In,Ga)Se₂ solar cell absorbers</i>
11:30 – 12:10	Michael Lorke, University of Bremen, Germany <i>Carbon in GaN revisited</i>
12:10 – 12:50	<i>Closing words: Thomas Frauenheim</i>
12:50	Departure