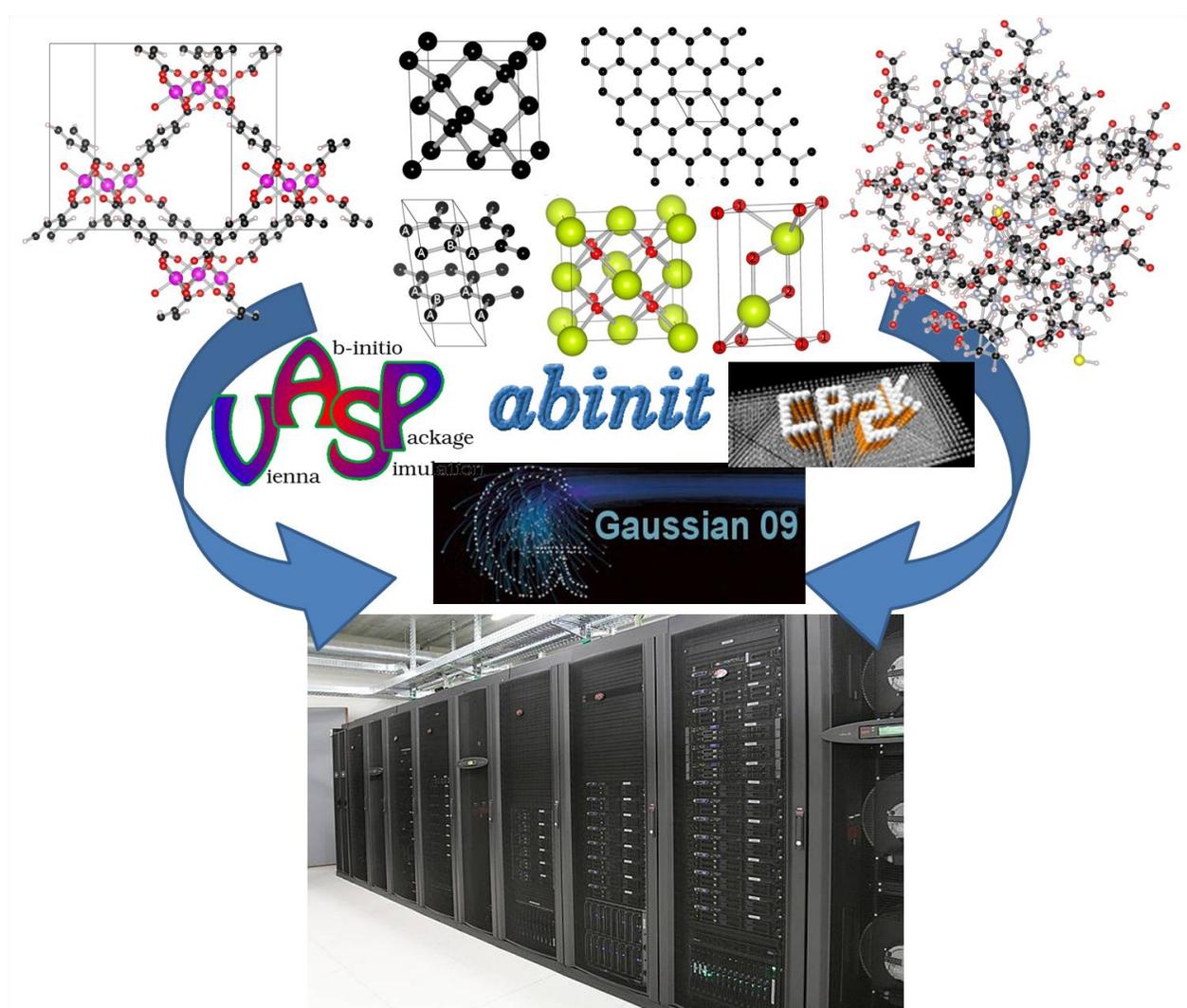# Spring School
Computational Tools for Materials Science

Ghent University
April 13th to 17th 2015

Campus Sterre, Krijgslaan 281, building S9,
auditorium A2-A3, 9000 Ghent, Belgium

Organization

This spring school is organized by the Center for Molecular Modeling (CMM) of Ghent University in collaboration with the Flemish Supercomputer Centre (VSC).

Dr. ir. Kurt Lejaeghere	(CMM, UGent)
Dr. Dr. Danny E.P. Vanpoucke	(CMM, UGent)
Prof. Dr. ir. Veronique Van Speybroeck	(CMM, UGent)
Mr. Wim Dewitte	(CMM, UGent)
Dr. Ewald Pauwels	(VSC, UGent)
Jan Ooghe	(VSC, KULeuven)
Dr. Stefan Becuwe	(VSC, UAntwerp)
Rosette Vandenbroucke	(VSC, VUB)
Prof. Dr. Dr. Geert Jan Bex	(VSC, UHasselt)

Scientific Advisory Committee

Prof. Dr. Stefaan Cottenier	(Center for Molecular Modeling, UGent)
Prof. Dr. Patrick Bultinck	(Ghent Quantum Chemistry Group, UGent)
Prof. Dr. ir. Xavier Gonze	(Nanoscopic Physics group, UCL)
Prof. Dr. Dipl.-Ing. Georg Kresse	(Computational Materials Physics group, University of Vienna)

Sponsors

Practical Information

- General information regarding the spring school is available on the webpage:
  https://molmod.ugent.be/spring-school-computational-tools-materials-science
- Exercise handouts and supplementary information can be downloaded from:
  https://molmod.ugent.be/owncloud/index.php/s/iHQ1rIbIQiYp8Rc
- You can log into your vsc-account (to join groups/upload keys/…) via:
  https://account.vscentrum.be/
- If you are staying in Ghent during the week, and are interested to visit the city (after the workshop) you will find useful information on this webpage: http://www.visitgent.be/

Program

Day-1: Basic Concepts in Computational Materials Science

9h00	**A2**	**Welcome & Introduction**	
			Prof. Dr. ir. Veronique Van Speybroeck
9h30	**A2**	**Session 1: Molecular Modeling**	
			Prof. Dr. ir. Karen Hemelsoet
11h15	**A3**	Coffee Break	
11h30	**A2**	**Session 2: Density Functional Theory**	
			Prof. Dr. Stefaan Cottenier
12h30	**A3**	Lunch	
13h30	**A2**	**Session 3: Solid State Modelling**	
			Prof. Dr. Stefaan Cottenier
14h30	**A2**	**Session 4: accessing the UGent HPC infrastructure**	
			Jens Timmerman
15h00	**A3**	**Poster Session & Reception**	
17h00		End of the first day	

Day-2: The VASP code

9h00   **A2**   **Session 1: a Bird's eye view of VASP**

<div align="right">Dr. Dr. Danny Vanpoucke</div>

10h15   **A3**   Coffee Break

10h30   **A3**   **Hands-on 1 session : Getting Introduced to VASP**

         Dr. ir. Kurt Lejaeghere, Dr. Dr. Danny Vanpoucke, ir. Michael Sluydts, Jan Jaeken, ir. Lennart Joos

12h30   **A3**   Lunch

13h30   **A2**   **Session 2: the Bethe-Salpeter equation and GW**

<div align="right">Dr. Martijn Marsman</div>

15h15   **A3**   Coffee Break

15h30   **A3**   **Hands-on 2 session : Kicking VASP into Gear**

         Dr. Martijn Marsman, Dr. ir. Kurt Lejaeghere, Dr. Dr. Danny Vanpoucke, ir. Michael Sluydts, Jan Jaeken, ir. Lennart Joos

17h00   End of the second day

Day-3: The ABINIT code

9h00   **A2**   **Session 1: a Bird's eye view of ABINIT**

         Prof. Dr. ir. Xavier Gonze & Dr. Matteo Giantomassi

10h15   **A3**   Coffee Break

10h30   **A3**   **Hands-on 1 session : Getting Introduced to ABINIT – From silicon to aluminum**

         Prof. Dr. ir. Xavier Gonze, Prof. Dr. ir. Gian-Marco Rignanese, Dr. David Waroquiers, Dr. Matteo Giantomassi

12h30   **A3**   Lunch

13h30   **A2**   **Session 2: Vibrational, dielectric and mechanical properties from density-functional perturbation theory**

         Prof. Dr. ir. Gian-Marco Rignanese & Prof. Dr. ir. Xavier Gonze

15h15   **A3**   Coffee Break

15h30   **A3**   **Hands-on 2 session : Aluminum Arsenide – from ground state to phonon band structure**

         Prof. Dr. ir. Xavier Gonze, Prof. Dr. ir. Gian-Marco Rignanese, Dr. David Waroquiers, Dr. Matteo Giantomassi

17h00   End of the third day

Day-4: The Gaussian code

9h00 **A2** **Session 1: a Bird's eye view of Gaussian**

ir. Dietmar Hertsen

10h15 **A3** Coffee Break

10h30 **A3** **Hands-on 1 session : Getting Introduced to Gaussian**

ir. Hannelore Goossens, ir. Dietmar Hertsen, Dr. Sofie Van Damme, ir. Pieter Cnudde, Dr. ir. Jeroen Van der Mynsbrugge, ir. Steven Vandenbrande

12h30 **A3** Lunch

13h30 **A2** **Session 2: Advanced concepts in Gaussian: from full CI to CAS-SCF**

Prof. Dr. Patrick Bultinck

15h15 **A3** Coffee Break

15h30 **A3** **Hands-on 2 session : Advanced concepts in Gaussian**

Dr. Sofie Van Damme, ir. Dietmar Hertsen, ir. Hannelore Goossens, Dr. ir. Pieter Cnudde, ir. Jeroen Van der Mynsbrugge, ir. Steven Vandenbrande

17h00 End of the fourth day

Day-5: The CP2K code

9h00 **A2** **Session 1: a Bird's eye view of CP2K**

Dr. ir. Andy Van Yperen-De Deyne

10h15 **A3** Coffee Break

10h30 **A3** **Hands-on 1 session : Basics of Molecular dynamics in CP2K**

Dr. ir. Andy Van Yperen-De Deyne, ir. Thierry De Meyer, ir. Lennart Joos, , ir. Pieter Cnudde, Dr. ir. Jeroen Van der Mynsbrugge

12h30 **A3** Lunch

13h30 **A2** **Session 2: QM/MM and TD-DFT applied to the ethyl orange dye**

ir. Thierry De Meyer

14h15 **A2** **Session 3: vibrational spectroscopy and fingerprinting**

Dr. ir. Andy Van Yperen-De Deyne

15h00 **A2** **Session 4: Integrating different codes: Unchain my Zeolite**

ir. Lennart Joos

15h20 **A3** Coffee Break

15h35 **A3** **Hands-on 2 session : MD analysis and QM/MM simulations**

Dr. ir. Andy Van Yperen-De Deyne, ir. Thierry De Meyer, ir. Lennart Joos, , ir. Pieter Cnudde, Dr. ir. Jeroen Van der Mynsbrugge

17h00 **A3** **Closing remarks**

Dr. Dr. Danny Vanpoucke & Dr. ir. Kurt Lejaeghere

17h15 End of the last day

Posters

#	Title	Presenter
1	Theoretical investigation on the radical polymerization of cellulose units with methyl acrylate	Suzan Abdurrahmanoglu & S. Erdem
2	Size dependent strain and surface energies of icosahedral and cuboctahedron gold nanoclusters: A computational study	Shahid Ali, V. S. Myasnichenko & E. C. Neyts
3	The time scale associated with Monte Carlo simulations	Kristof Bal & E. C. Neyts
4	Exploiting click-chemistry to modify an allyl Periodic Mesoporous Organosilica into FiLiUSS	Sander Clerick, E. De Canck & P. Van Der Voort
5	Ab initio study of methyl radical and benzene adsorption on α-Cr_2O_3 (0001) surfaces: The role of van der Waals density functionals.	Samira Dabaghmanesh, E. C. Neyts & B. Partoens
6	Theoretical Investigation of Electronic Structures and Properties of Silicon-doped Boron Clusters	Thi Tuyet Mai Dang & M. T. Nguyen
7	Triazolinediones enabling click and transclick reactions	Kevin De Bruycker, S. Billiet, H. Houck, F. Driessen, H. Goossens, V. Van Speybroeck, J. M. Winne & F. E. Du Prez
8	Persistent luminescent nanoparticles with applications for in vivo imaging	Olivier De Clercq, P. F. Smet, & D. Poelman
9	Thermal Expansion Coefficients of Ni, Pt and Pd Germanides and Silicides	Filip Geenen, W. Knaepen, F. Moens, L. Brondeel, A. Leenaers, S. Van den Berghe & C. Detavernier
10	Modeling aldol condensations in UiO-66 type materials	Julianna Hajek, M. Vandichel, F. Vermoortele, M. Waroquier, D. De Vos & V. Van Speybroeck
11	The nature of α-Fe in Fe-ZSM-5	Simon Hallaert, P. Vanelderen, K. Pierloot, B. Sels & R. Schoonheydt
12	Adsorption of C and CH_x radicals on anatase (001) and the influence of oxygen vacancies	Stijn Huygh & E. C. Neyts
13	From Accurate Models to Zero Emissions	Lennart Joos, B. Smit & V. Van Speybroeck
14	Designing phosphors for brighter LEDs	Jonas Joos, D. Poelman & P. F. Smet
15	thINK outside the box	Wouter Marchal, G. Vandevenne, K. Elen, W. Deferme, M. Van Bael & A. Hardy
16	Microwave assisted synthesis of mesoporous titania and relevant surface interactions with dye molecules	Mieke Meire, P. Van Der Voort, I. van Driessche & P. Lommens
17	Synthesis, properties and modeling of doped ZnO nanostructures	Aleksandr Momot, M. Amini, A. Volodine, K. Elen, M. Van Bael & A. Hardy

18	Periodic mesoporous organosilicate thin films for low-k application	Murad Redzheb, M. Baklanov & P. Van Der Voort
19	A Multi-Scale Modelling Platform applied towards Fischer Tropsch Synthesis on Fe catalysts	Jose Rivera De La Cruz, M.-F. Reyniers & G.B. Marin
20	Design of Pt-based catalysts for the catalytic dehydrogenation of propane	Stephanie Saerens
21	What is a superaromat? Calculations on C50	Ana Sanz Matias, A. Ceulemans & M. Alcami
22	High throughput first-principles calculations of bixbyite oxides for TCO application	Nasrin Sarmadian, R. Saniz, B. Partoens, D. Lamoen, K. Volety, G. Huyberechts & J. Paul
23	Modelling of polymer composites at the nanoscale	David Seveno, A. Ostadhossein & A. Van Duin
24	Ab initio high-throughput study of extrinsic point defects in Si and Ge	Michael Sluydts, J. Vanhellemont, V. Van Speybroeck & S. Cottenier
25	Qualitative insights into transmission probability through molecular electronic devices	Thijs Stuyver, S. Fias, F. De Proft & P. Geerlings
26	Computational Investigation of New Potent Antagonists for the Glycine Binding Site of N-Methyl-D-Aspartate (NMDA) Receptor	D. Akgül, Gamze Tanriver, G. Çifci, Ş. Çatak & V. Aviyente
27	Effects of cation attachment on the singlet-triplet gap and bonding of silicon trimer	Tran Dieu Hang, N. M. Tam, H. T. Pham, M. P. Pham-Ho & M. T. Nguyen
28	Triazolinediones as a rapid functionalization and crosslinking tool for plant oil based step-growth polymers	Laetitia Vlaminck, K. De Bruycker, O. Turunc, S. Ouardad & F. E. Du Prez
29	Computational tools to accelerate the development of novel functional biobased materials	Aleksandra Wróblewska, S. De Wildeman & Katrien Bernaerts
30	Atomic scale simulations of plasma interactions with model systems for plasma medicine	Maksudbek Yusupov, J. Van der Paal, E. C. Neyts & A. Bogaerts

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