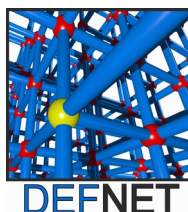


DEFNET-641887



MSCA-ITN-2014-ETN



Horizon 2020



DEFNET
(Grant Agreement No: 641887)
DEFect NETwork Materials Science and Engineering
DEFNET Workshop 3: Theory and Spectroscopy

Tuesday, March 22, 2016

- 8:50 - 9:00 Workshop Opening, Veronique Van Speybroeck (UGent)
- 9:00 - 10:00 **Theory:** Introduction to theoretical methods for calculating structure and properties of framework materials, Veronique Van Speybroeck (UGent)
- 10:15 - 11:15 **Theory:** Link between theory and practical aspects of DFT calculations with VASP, An Ghysels (UGent)
- 11:30 - 14:45 **Hands-on session** & lunch: Structural stability of flexible MOFs in VASP, Kurt Lejaeghere, Jelle Wieme, Arthur De Vos, Michaël Sluydts (UGent)
- 15:00 - 17:00 Poster session

Wednesday, March 23, 2016

- 9:00 - 10:00 **Theory:** Overview of force-field models and molecular dynamics simulations with periodic boundary conditions, Toon Verstraelen (UGent)
- 10:15 - 11:15 **Theory:** How to estimate the unknown parameters of molecular mechanics force fields, Louis Vanduyfhuys (UGent)
- 11:30 - 12:30 **Theory:** ReaxFF overview, Ole Carstensen (SCM)
- 12:30 - 13:30 Lunch break
- 13:30 - 17:00 **Hands-on sessions:**
- Using QuickFF to derive force fields for framework materials, Louis Vanduyfhuys, Steven Vandenbrande (UGent)
 - ReaxFF applications and analysis, Ole Carstensen (SCM)
- 19:00 - ... Social Dinner

Thursday, March 24, 2016

- 9:00 - 10:00 **Theory:** Zooming in on Defects: QM/MM, Rochus Schmid (RUB)
- 10:00 - 10:30 **Theory:** UHV-FTIR spectroscopy on defect-engineered MOFs, Yuemin Wang (RUB)
- 10:45 - 12:00 **Theory:** ADF overview, Mirko Franchini (SCM)
- 12:00 - 13:00 Lunch break
- 13:00 - 17:00 **Hands-on sessions:**
- Application of a QM/MM approach to compute the IR signatures of probe molecules in (defect) MOFs, Rochus Schmid, Roberto Amabile, Johannes P. Dürholt (RUB)
 - ADF spectroscopy applications, Mirko Franchini (SCM)