A.D. 1308
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DIPARTIMENTO
DI INGEGNERIA
CIVILE E AMBIENTALE
DIPARTIMENTO DI ECCELLENZA

CIVIL AND ENVIRONMENTAL ENGINEERING

DOCTORAL PROGRAM 2020-2021

Dr Stefano Leoni is Associate Professor in the School of Chemistry, Cardiff University since 2013. He holds a PhD from ETH Zurich, Switzerland. Previously, he was Assistant Professor and Group Leader of an externally funded research group at Dresden University of Technology, Germany (2010-2013), and distinguished Heisenberg Research Fellow (2013- 2016) of the Deutsche Forschungsgemeinschaft (DFG). These positions followed a 10-year appointment at the Max-Planck Institute for Chemical Physics in Dresden, Germany (2000- 2010), where he obtained his Habilitation (venia legendi) in 2009 with a thesis on novel advanced molecular dynamics techniques applied to simulate reconstructive phase transitions. From 2004 to 2006, he was awarded an Advanced Research Fellowship of the Swiss National Foundation (SNF). In 2013, he was appointed Adjunct Professor at the University of Bern, Switzerland.

Location

Teams platform - CEEPhD Team (Room 2)

https://teams.microsoft.com/l/meetup-join/19%3ae92fb49e755f457a8faff0a30c561bf1%40thread.tacv2/1634210278254?context=%7b%22Tid%22%3a%22067e7d20-e70f-42c6-ae10-8b07e8c4a003%22%2c%22Oid%22%3a%22fa19f6c2-6b18-4de4-b45f-3c8b36015efd%22%7d

Timetable

October, 18th 2021, from 10:00 to 13:00,
from 14:00 to 17:00 CET
October, 20th 2021, from 10:00 to 13:00 CET
October, 22nd 2021, from 14:00 to 17:00 CET
November, 3rd 2021, from 10:00 to 13:00,
from 14:00 to 17:00 CET
November, 5th 2021, from 10:00 to 13:00,
from 14:00 to 17:00 CET

MOLECULAR DYNAMICS METHODS AND SIMULATION STRATEGIES FOR ENERGY MATERIALS

Instructor

Stefano Leoni, Associate Professor, School of Chemistry, Cardiff University

Course Description

This course aims at giving an overview of molecular dynamics methods, including advanced techniques for enhanced sampling, free energy calculations, and the impact of machine learning on interatomic potentials. This will be accompanied by in-depth discussions of their application to relevant areas of energy conversion, storage and reactivity in materials devices.

Course Schedule (24 hours, 4 CFU)

Monday Oct 18th 2021 (6 hours)
10:00 – 13:00 CET: Lecture 1 – MD, Foundation
14:00 – 17:00 CET: Workshop 1 – MD Simulations

Wednesday Oct 20th 2021 (3 hours)
10:00 – 13:00 CET: Lecture 2 – MD, Advanced techniques

Friday Oct 22nd 2021 (3 hours)
14:00 – 17:00 CET: Workshop 2 – Advanced MD Simulations

Wednesday Nov 3rd 2021 (6 hours)
10:00 – 13:00 CET: Lecture3– Electronic and Phonon Transport
14:00 – 17:00 CET: Workshop 3 – Wannier Functions

Friday Nov 5th 2021 (6 hours)
10:00 – 13:00 CET: Lecture 4 – Electrochemical Storage
14:00 – 17:00 CET: Workshop 4 – Hubbard U and related tools, the role of correlation in Energy storage materials

For more info Mrs. Teresa Nocera, Ph.D. Program Secretariat (teresa.nocera@unipg.it)
Prof. Dr. Filippo Ubertini, Ph.D. Program Coordinator (filippo.ubertini@unipg.it)

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