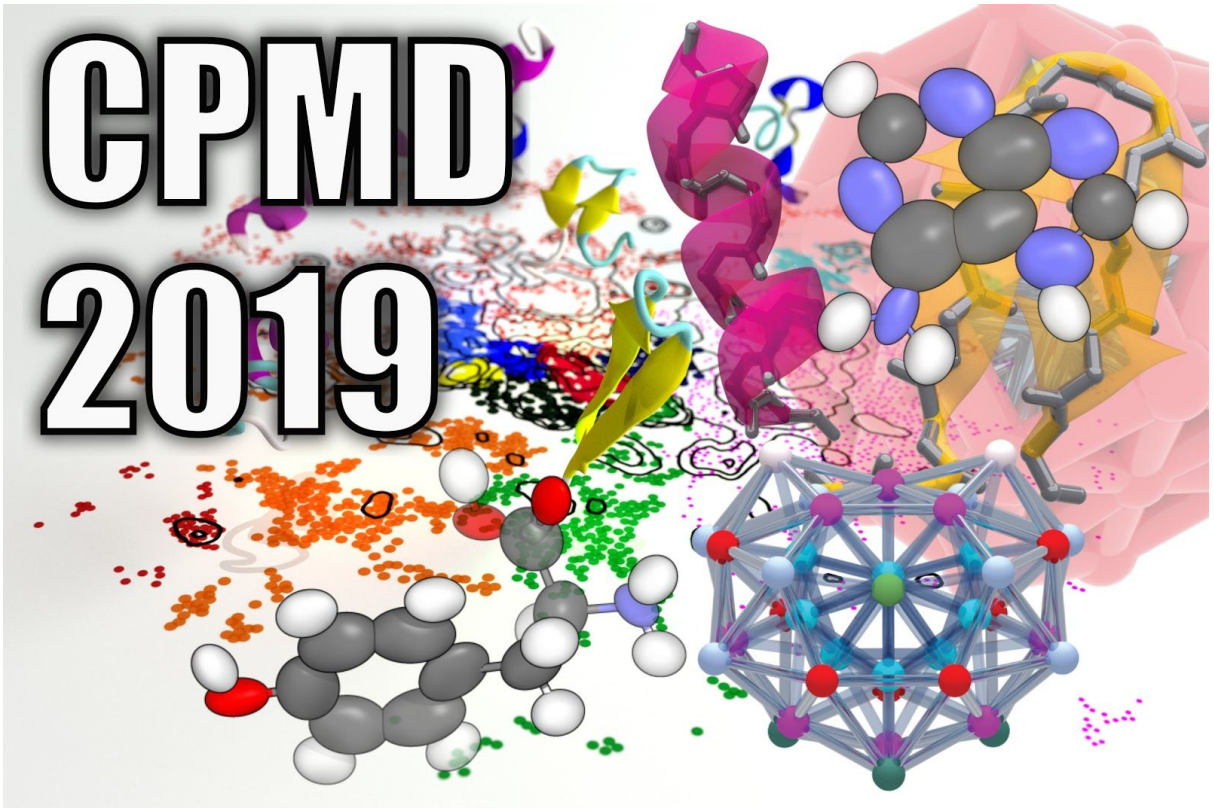
Scientific report on the CPMD 2019 Meeting
Pushing the Boundaries of Molecular Dynamics
CECAM-HQ-EPFL, Lausanne, Switzerland
July 22, 2019 – July 24, 2019



CPMD meetings have a tradition stretching back two decades in bringing together a diverse mix of computational scientists working on different aspects of molecular dynamics simulations, combining aspects of electronic structure theory and statistical sampling methods, as well as state-of-the-art applications ranging from materials science to biophysics.

This edition of the meeting – which marked the 20th anniversary of the first CPMD meeting at Ringberg Castle (Munich) – focused on identifying the most pressing challenges in the field, and on discussing the most promising directions to face such challenges. Given the growing relevance of machine-learning methods in the field of atomic-scale modelling, the topic was given a particular focus, informed the choice of the speakers and the organization of the program.

A total of 24 speakers presented oral contributions, while 46 participants presented a poster. The meeting was attended by a total of 95 participants (including organizers and speakers) from 19 countries. Full details of the program can be found on https://www.cecam.org/workshop1738/ and on https://sites.google.com/view/cpmd-2019/home.

Organizers
Michele Ceriotti (EPFL)
Nicola Marzari (EPFL)

Matteo dal Peraro (EPFL)
Alfredo Pasquarello (EPFL)

Sponsors

CPMD 2019 was funded by CECAM, Psi-k, and MARVEL

Scientific scope

The meeting has seen a broad overview of the state of the art in atomic-scale modelling of materials and molecules. While machine learning has been a recurring theme, it has been presented not as an end in itself, but considered in the broader context of the challenges faced by molecular dynamics simulations. Three distinct perspectives emerged:

1. **Pushing the boundaries for electronic structure methods in ab initio molecular dynamics.** With the advent of machine-learning potentials, it becomes even more crucial to provide very accurate reference values, that can be used not only for direct sampling, but also to train surrogate quantum models. During the meeting we saw several examples of simulations that use beyond-DFT methods, and high-performance computing optimization to enable more accurate and/or lower-cost electronic structure calculations to be used in AIMD simulations.
2. **Data-based science and machine learning.** Speakers presented several new developments in the application of data-driven techniques to atomistic modelling. These developments are changing the landscape of molecular modelling — for instance through the development of machine-learning potentials, the design of optimal descriptors to predict material properties, and the automatic determination of order parameters for sampling
3. **Pushing the boundaries for sampling, and long time-scale modelling**. Several approaches were presented to compute more accurate free-energies for both stable phases, reactive events, and conformational changes in proteins, including effective thermostatting schemes, replica exchange methods, nested sampling, and biased sampling algorithms.

List of speakers and talks:

Alessandro Curioni, IBM Research Europe
My take on molecular simulations for materials design: past, present and future

Mariana Rossi, FHI Berlin
Structure and Dynamics of Molecular Crystals

Christoph Dellago, University of Vienna
Fluctuating interfaces and the bulk melting of ice

Yoshitaka Tateyama, NIMS Tsukuba
DFT sampling approach of interface and surface processes in battery and catalyst

Yi Qin Gao, Peking University
Dynamic Electric Field Effects on Claissen Rearrangement Reaction

Fabio Pietrucci, Sorbonne University Paris
Towards a general approach to chemical reactions in solution

Roger Rousseau, PNNL
Theoretical mechanistic studies of electrochemical hydrogenation of organic compounds

Omar Valsson, MPI Mainz
Recent Developments and Applications of Variationally Enhanced Sampling

James Kermode, University of Warwick
Multiscale QM/MM modelling of rare events in materials chemomechanics

Giulia Galli, University of Chicago
Sorting through messy solids and liquids with first principles molecular dynamics

Michiel Sprik, Cambridge
From electrode to interface potentials

Marcella Iannuzzi, University of Zurich
Molecules at the Electrochemical interface: Understanding Experiments with Simulations

Oliviero Andreussi, University of North Texas
Continuum Approaches in Electrochemistry

Michele Vendruscolo, Cambridge
Principles of Protein Structural Ensembles Determination

Luca Ghiringhelli, FHI Berlin
Charting spaces of materials properties

Giovanni Piccini, ETH Zurich/USI
Enhancing efficiency and accuracy in chemical reactions sampling

Ali Hassanali, ICTP Trieste
Wild Fluctuations in Liquid Water

Chris Mundy, PNNL
Ions in aqueous solution: From intrinsic to collective properties

Akihiro Morita, Tohoku University
Microscopic Dynamics and Kinetics at Liquid-Liquid Interfaces

Sara Bonella, EPFL
Zero mass constraints for the evolution of adiabatically separated systems

Mike Finnis, Imperial College London
Calculation of high-temperature properties of ZrC and MAX phases

Livia Bartók-Partay, University of Reading
Nested sampling for exploring potential energy landscapes

Jutta Rogal, Bochum University
Path collective variables for enhanced sampling of structural phase transformations

Federico Grasselli, SISSA Trieste
Topological quantisation and gauge invariance of charge transport in liquid insulators