POSTER SESSION

Search for a new water-splitting catalyst using molecular dynamics simulations based on CCSD(T) and DFT data
Omololu Akin-Ojo

Performance evolution of FLEUR
Uliana Alekseeva

Overview of SIESTA developments within the MaX project
Jose Miguel Alonso Pruneda

Electronic and Optical Properties of Hydrogen Doping in Anatase Titania
Samaneh Seyedeh Ataei

Excited states in TiO2
Michael Atambo

Ab-initio Calculations of Oxygen Reduction on High-Index Platinum Surfaces
Seyedjavad Azimigehraz

Structural, electronic and optical properties study of the cubic phase of the halide perovskyte CsSnBr3 using DFT calculations
Karima Benyahia

A non-conventional use of AiiDA: validation and performance evaluation of Quantum ESPRESSO on different HPC architectures
Marco Borelli

KKRnano: Density Functional Theory application for a million atoms
Marcel Bornemann

The AiiDA-FLEUR package
Jens Bröder

Alternative Materials For Plasmonics In The Near-IR And Visible Range
Arrigo Calzolari

Spin-Orbit implementation by means of fully separable Kleinman-Bylander pseudopotential formalism under an atomic orbital basis in SIESTA code
Ramón Cuadrado Del Burgo

Thermo_pw: a FORTRAN driver for Quantum ESPRESSO routines
Andrea Dal Corso

SIESTA interface to AiiDA
Vladimir Dikan

AiiDA - Automated interactive infrastructure and database for computational science
Sebastiaan Huber

Linear Response with Density Functional Perturbation Theory in SIESTA
Sergio llera

A performance study of Quantum ESPRESSO's diagonalization methods on cutting edge computer technology for high-performance computing
Anoop Chandran Kaithalikunnel

Calculation of properties of magnetic materials using a high throughput framework for Korringa-Kohn-Rostoker Green function method
Roman Kováčik

Realising the Impact of Fluorination on Potential Window of Carbonate Electrolytes in Li-ion Battery: A First Principles Investigation
Anoop Kushwaha

Evaluation of topological numbers within hybrid functionals
Hyungjun Lee

Accelerating Crystal Structure Prediction using ab-initio data and Deep Neural Networks Force Fields Ruggero Lot

Prediction of a large-gap and switchable Kane-Mele quantum spin Hall insulator
Antimo Marrazzo

GW calculations without massive use of empty states: a new tool in Yambo
Ivan Marri

Large scale quantum Monte Carlo simulations for materials at planetary conditions
Guglielmo Mazzola

Coupling of i-PI and ONETEP codes to enable petaScale simulations for first principles modelling of both electrons and nuclei for thousands of atoms
Elliot Menkah

MD-based characterization of plastic deformation in Cu/Ag nanocomposites via dislocation extraction analysis
Abbas Montazeri Hedesh

CO2 Adsorption on TiO2 Anatase (001) Activated by Oxygen Vacancies
Javier Montoya Martínez

Magnetic coupling on molecular interfaces with high thermal stability
Claudia Maria Pereira Cardoso

High Energy Density Supercapacitor Electrode Based on Vanadium Selenide reduced Graphene Oxide Hybrid
Satyajit Ratha

Hybrid QM/MM simulations of electronic transport in aqueous solutions
Alexandre Reily Rocha

Challenges in automated high-throughput ab initio calculation in magnetic materials
Matti Ropo

Multi scale computational approach to the study of gold nanocluster properties in different solvents Marta Rosa
First principles study of vertical spin switch in atomic scale two-dimensional system
Mihir Sahoo

Investigatio of lithium-ion solvation and diffusion in ethylene carbonate using classical molecular dynamics
Nnanna Ukoji

Clean Os(0001) electronic surface states: a first-principle fully relativistic investigation
Andrea Urru

Large-Scale Implementation of the Density Matrix Renormalization Group Algorithm
James Vance

Carbon nanotubes as excitonic insulators
Daniele Varsano

Growth Mechanism of Small PdGa Bimetallic Clusters on MgO (100) Surface
Nandhakumar Velankanni

Automation of Maximally Localised Wannier functions for high throughput calculations via the selected column of the density matrix algorithm (SCDM-k) in Wannier90
Valerio Vitale

Half-Heusler ZrFeSi: Efficient Thermoelectric material
Saleem Yousuf

Lithium interactions with graphene at finite temperature
Yusuf Shaidu