CECAM Workshop Outbox October 7th -11th, 2019 _ Poster Presentations

Name	Firstname	Topic
Balzaretti	Filippo	From ab-initio to experiments: how to clean water via Rutile TiO2
Bisbo	Malthe Kjær	Efficient global structure optimization with machine learned surrogate potential
Bissuel	Dylan	Towards DFTB repulsive potentials using neural-networks
Camacho	Cristopher	A GPU-accelerated implementation of DFTB+
Chagas da Silva	Mauricio	Modeling substitutional defects and electronic features in goethite mineral: a machine learning approach
Chiriki	Siva	Global optimization of Pt clusters on Al2O3 (0001) surface using Gaussian process regression
Chou	Chien-Pin	Density-functional tight-binding metadynamics study of oxy-carbon diffusion on (100)-γ-Al2O3 surface
Christensen	Anders S.	Operators in machine learning: response properties in chemical space
Coutinho Neto	Maurício D.	A simple polarizable classical force field to describe water/metal interfaces
Domínguez-Castro	Adrian	Ehrenfest dynamics simulations of laser-induced CO photooxidation onto TiO2 anatase
Ehlert	Sebastian	A robust and broadly parametrized non-selfconsistent tight binding quantum chemistry method for extended systems
Gupta	Verena Kristin	Coadsorption of water and nitric oxide on anatase TiO2
Heinen	Stefan	Machine learning the computational cost of quantum chemistry
Kapetanovic	Edin	Extended Hubbard Model with nearest neighbor exchange interaction
Khorasani	Elham	Testing the HSE functional for defects in layered van der Waals materials
Krämer	Mila	Machine-learning coarse-grained hamiltonians for unbiased electron and exciton dynamics simulations
Kromann	Jimmy Charnley	A python framework for quantum machine learning
Li	Xinyu	Improved description of catalysis adsorption using machine learning
Maity	Sayan	QM/MM Molecular dynamics simulations of the FMO light-harvesting complex using the TD-LC-DFTB approach
Margraf	Johannes T.	Predicting the thermochemistry of large reaction networks with machine learning
McSloy	Adam	Towards a machine-learning-based DFTB parametrisation for hybrid metal-organic systems
Medrano Sandonas	Leonardo	Transferable and robust DFTB repulsive potentials from neural networks

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Meldgaard	Søren A.	Machine learning enhanced global optimization by clustering local environments
Mortensen	Henrik L.	Atomistic structure learning
Nishimura	Yoshifumi	Hierarchical parallelization of DFTB simulations with DCDFTBMD
Ono	Junichi	Long-time quantum molecular dynamics simulations based on divide-and-conquer density-functional tight-binding method for sodium-ion transport in electrolyte solutions
Petersen	Thorben	Excited state wave-packet dynamics study of water oxidation on ideal TiO2-anatase(101)
Posenitskiy	Evgeny A.	Competition between ultrafast relaxation in UV-excited tetracene and chrysene
Prajapati	Jigneshkumar Dahyabhai	Minimum free energy pathways of ciprofloxacin and enrofloxacin across a bacterial pore
Röhr	Merle I. S.	Metadynamics for automatic sampling of quantum property manifolds (ASQPM)
Santana-Bonilla	Alejandro	STK: a vesatile python tool for a first-principle database creation
Schüler	Malte	Combining DFT with model based approaches for nano-structured systems with strong electronic correlations
Tahchieva	Diana N.	Nine thousand carbenes: ML of accurate spin gaps, strong correlation, and chemical insights
Teusch	Thomas	Water oxidation on WO3(001) – an embedded cluster study supported by machine learning
van Loon	Erik	Coulomb engineering of two-dimensional Mott insulators
Verner Christiansen	Mads-Peter	Complimentary energy landscapes for global relaxation

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