



# EuroHPC Summit Week 2019

## Tuesday 14 May 2019

### PRACEdays Scientific Track 4: Materials & Chemistry - Room F (17:00-19:00)

**-Conveners: Matej Praprotnik**

time	[id] title	presenter
17:00	[23] Modelling mechanism of reactions and active sites in heterogeneous catalysis, looking for reactivity indicators in supported ziegler-natta nano-systems	D'AMORE, Maddalena
17:30	[24] Silica for drug-delivery: when simulation can complement experiment	DELLE PIANE, Massimo
18:00	[25] Shear rheology of polymer melts and nanocomposites via nonequilibrium molecular dynamics simulations	TSALIKIS, Dimitrios
18:30	[26] The peptide bond condensation reaction at the air/water interface catalyzed by the "salt of the life"	SIRO BRIGIANO, Flavio