Multiscale phenomena in molecular matter

Thursday 6 July 2017

Computational Physics (11:30 - 13:40)

-Conveners: Zbigniew Łodziana

time	[id] title	presenter
11:30	[47] Electrochemical reduction of NO on Pt(100): a combined DFT and KMC study	Prof. HONKALA, Karoliina
12:00	[53] Challenges in the modelling of oxides	Prof. LOPEZ, Nuria
12:30	[78] Spin transition of Fe(II) 1D triazole chains: hybrid materials and lattice dynamics	Prof. GARCIA, Yann
13:00	[32] Structural phase transition in KFe$_2$As$_2$ from ab initio calculations	Dr STERNIK, Małgorzata
13:20	[45] Hydrogen in AB$_2$ and AB$_5$ compounds	Dr BUDZIAK, Andrzej