

Table of contents

Wednesday 16 February 2022	1
----------------------------------	---

Second Adriatic Conference on Strongly Correlated Systems (and beyond) | (smr 3688)

Wednesday 16 February 2022

Numerical simulation of quantum materials - Online (09:15-12:00)

Chairperson: Giuliano CHIRIACÒ (ICTP, Italy)

time	title	presenter
09:15	Introductory talk to Density Functional Theory	NICOLA SERIANI
10:00	Unraveling the catalytic and photocatalytic decomposition of N ₂ O on Titanium dioxide based material: a DFT+U study	ELHAM MOHARRAMZADEH GOLIAEI
10:20	Kane-Mele and emergent topology in novel materials: from computational discovery to materials design	ANTIMO MARRAZZO
10:40	Coffee break	
11:00	The phase diagram of iron from quasi-ab initio calculations	ZHI LI
11:20	A flexible neural-network interatomic potential for mixed ionic materials: from bulks to clusters and nanoparticles	SAMARE ROSTAMI
11:40	An unsupervised approach for studying free energy landscapes characterized by order-disorder transitions	GIULIA SORMANI