



# ADVANCED MATERIALS AND NANOTECHNOLOGY

SEMINAR SERIES 2020

CEITEC - BRNO UNIVERSITY OF TECHNOLOGY  
LARGE MEETING ROOM

## Prof. Michele Pavone

*Universita' degli studi di Napoli, Italy*

### Design of heterogeneous functional materials for energy conversion: a quantum chemical perspective

**May, 19**

**Tuesday, 10:00**

Seminar room **S2.02**

CEITEC BUT Purkynova 123

**Invited by:**

Dipl.-Ing. Dr.techn.Hermann  
Detz

Global advances in industrialization are precipitating the rapid consumption of fossil fuel resources with increasing levels of atmospheric greenhouse gases. After the UN international conference on climate change (Paris 2015) and despite the recent political shift in USA, there is a worldwide consensus on implementing all possible actions to dislodge our dependence on oil, coal and natural gas. World sustainability requires viable sources of renewable energy and new technologies for its efficient conversion into commodities such as fuels or electricity.

Material Sciences play a pivotal role in optimizing the functional materials that are at the core of energy conversion devices. This is not a trivial task. The conversion of energy is the result of several physical and chemical processes that involve chemical reactions, charge and mass transport occurring across heterogeneous interfaces. Often, experimental techniques cannot dissect subtle features at the nanoscale that can hinder an effective design of new devices. Thus, the application of computational modeling tools with atomistic resolution represents an ongoing revolution in materials design and device development.