



UNIMORE
UNIVERSITÀ DEGLI STUDI DI
MODENA E REGGIO EMILIA

Dipartimento di Scienze Fisiche,
Informatiche e Matematiche



FIM-S3 SEMINAR

Alkali metal (Li, Na, K) ion battery electrodes and optical properties of van der Waals solids from first-principles calculations

Wednesday April 24th, 2024 – 16.00 (sharp)

S3 Seminar Room, 3rd Floor, Physics building

Speaker

Burak OZDEMIR – Unimore

Abstract

Na and K metals are more abundant and ubiquitous in nature compared to Li, therefore it is important to find suitable materials which can be intercalated with these metal ions for battery application. Conventional Li-ion battery anode graphite can not be intercalated with Na even though it is possible to intercalate it with Li. We show that graphite can be intercalated with K instead of Na with considerable specific capacity and it has suitable voltage for battery anodes. In order to intercalate graphite with Na, boron doping of graphite such as BC₃ can be used. Moreover, transparency of nanoscale few-layer graphene increases significantly with K intercalation and therefore it can be used as a smart-window in energy saving buildings. K intercalation of few-layer graphene increases the transparency much more than Li. In the first-principles calculations of alkali metal intercalation of layered materials, van der Waals correction is important. In the optical properties of van der Waals solids it is important to take into account the van der Waals interaction and in the case of alkali metal intercalated graphite, the contribution of intraband transitions as well as the interband transitions should be taken into account. It is essential to calculate plasmon resonance energy to understand optical properties of alkali metal intercalated graphite.

In collaboration with

