National University of Technology (NUTECH) Islamabad

A ONE DAY HANDS-ON WORKSHOP

DENSITY FUNCTIONAL THEORY APPROACH FOR SIMULATION OF PEROVSKITE MATERIAL PROPERTIES AND ENVIRONMENTAL STABILIZATION

Density functional theory (DFT) has been the dominant method for the quantum mechanical simulation of periodic systems for the past 40 years. It is the favorite choice of engineers, physics, and chemist in the past few years to simulation of energy materials, surfaces, molecules, and nano-scale electrical, electronic, optoelectronic, and photovoltaic devices. In this workshop, we introduce the basic concepts underlying density functional theory using the well-known DFT software packages such as SIESTA and VASP. This workshop is intended for the researchers with little or no experience of quantum mechanical simulations but with a basic undergraduate-level knowledge of quantum mechanics or electronic devices. Next, DFT simulation technique will be applied during the workshop to simulate

1. Atomic model/structure development like crystal growth/synthesis
2. Perovskite material properties and environmental stabilization for different operating condition

REGISTRATION:

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Email: cpd@nutech.edu.pk

25 NOVEMBER 2022
10 AM - 2 PM

NUTECH MAIN IJP ROAD
I-12, ISLAMABAD

CPD POINTS: 1.0

REGISTRATION FEE:

700 PKR /PERSON

LAST DATE TO REGISTER
23 NOVEMBER 2022

Dr. Muhammad Ejaz Khan has profound interest in organic-inorganic hybrid halide perovskites for solar cells and electronic devices. Moreover, he also has an experience of over a decade on simulation of nanostructures for industrial optoelectronic devices through density functional theory, force field, tight-binding, and effective mass approximation approaches.

Speaker

MUHAMMAD EJAZ KHAN

Associate Professor

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