



Seminarium Zakładu Energetyki Jądrowej i Analiz Środowiska (UZ3) Departament Badań Układów Złożonych (DUZ)

Wtorek: **11.04.2023**

11:30

transmisja online:

<https://www.gotomeet.me/NCBJmeetings/uz3-and-phd4gen-seminars>

Michał Komorowicz
NCBJ

Investigation of corrosion by means of adsorption energy analysis in DFT simulations

Abstract:

Corrosion is a complex phenomenon that can adversely affect the efficient functioning of various appliances, including a DFR reactor. Therefore, accurately predicting the corrosion rate and selecting appropriate resistant materials are crucial to ensure the longevity and reliability of such equipment. Investigating the adsorption energy of corrosive agents is one of the effective ways of predicting corrosion and comprehending the underlying behaviour of the process. In this regard, Density Functional Theory (DFT) simulations have been conducted to investigate the energy of lead adsorption on silicon carbide by different crystalline surfaces. Studies of this type often show promising results that are closely in line with experimental data. The primary objective of this work is to predict corrosion rates, which can aid in selecting appropriate resistant materials and confirm the validity of the choice of reactor material. Additionally, the study may provide valuable insights into mitigating corrosion. The presentation will cover the results and current status of ongoing simulations.

Serdecznie zapraszamy
Mariusz Dąbrowski, Tomasz Kwiatkowski
<http://www.phd4gen.pl>

Bio:

Michał Komorowicz is a PhD Student at National Centre for Nuclear Research. The primary focus of his research is to analyze corrosion in the DFR reactor. He is a member of a group dedicated to the development of a mini-demonstrator for this reactor.