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

Wtorek: **26.04.2022**
11:30

Michał Komorowicz

Ceramic corrosion study via molecular dynamics: Model development

Abstract:

The robustness and durability of materials are often a key limiting aspect of advanced technologies like the DFR reactor. When exposed to extreme conditions, even the most resistant materials degrade over time. The aim of this study is to create a molecular dynamics simulation using the LAMMPS environment and related software as an alternative to long and demanding laboratory tests. This model will allow studying the influence of liquid metal on ceramics at very high temperatures. Calculations on this scale require some unavoidable non-physical assumptions to get closer to reality. It is essential to apply an appropriate calibration that takes into account the choice of acceptable inaccuracies to meet achievable computation times. The talk will describe the development and current status of the ongoing work.

Serdecznie zapraszamy
M. Dąbrowski, T. Kwiatkowski
<http://www.phd4gen.pl>