SEMINAR NOTICE

Department of Physics and Engineering Physics
University of Saskatchewan

SPEAKER: Ali Abdolahzadeh Ziabari, PhD candidate,
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TOPIC*:* *Investigation of the Toxicity of the Materials Using ab initio Calculations*

DATE: Tuesday October 29th, 2024

TIME: 3:30-4:30 p.m.

PLACE: ***Physics 103***

Abstract:

To understand the toxic potencies of environmental pollutants, it is essential to explore the interaction between protein receptors and ligands. This study combines physico-chemical properties calculated via ab initio density functional theory (DFT) and molecular dynamics (MD) simulations to link molecular ligand-receptor binding to in vitro responses. We present our ongoing work, aiming to predict variations in aryl hydrocarbon receptor (AhR)-mediated toxic potencies among homologues of polychlorinated biphenyls (PCBs) with structural modifications. Our work involves DFT calculations of PCB molecules and MD simulations of the 4f3l receptor in complex with PCBs as ligands, as well as the CYP1B1-PCBs complex. CYP1B1, the enzyme responsible for monooxygenation, may lead to the formation of DNA adducts, which serve as reliable biomarkers for tumor cell metabolism.