# SEMINAR NOTICE

## *Department of Physics and Engineering Physics*
## *University of Saskatchewan*

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**SPEAKER:** Gap Soo Chang,
Department of Physics & Engineering Physics

**TOPIC***:* ***How a physicist approaches a problem of environmental*** **Bio-toxicity: Sabbatical research at Seoul National University in Korea**

**DATE:** Tuesday September 24th, 2019

**TIME:** 3:30-4:30 p.m.
**PLACE:** Physics 175

## ABSTRACT:

When a scientific problem is multifaceted and beyond the scope of a single discipline of research, an interdisciplinary approach to solving that problems is imperative. In this work, we brought research groups from physics and toxicology together to develop a predictive model for bioavailability and toxicity of organic chemicals. There are tons of chemicals in the environment that can activate the aryl hydrocarbon receptor (AhR) and thus cause toxicity. *In vivo* (animal) and *in vitro* (cell) studies have played a primary role in assessing adverse effects of chemical substances on bio-organisms for past decades. However, recent upsurge in new chemicals found or synthesized for industrial purposes outpaces the evaluation ability of these conventional methods which are highly cost- and labour-intensive. For example, in a single year of 2014, more chemical substances were added to CAS registry than in the combined years from 1965-1990 and a new substance is being added to the registry in every 9 seconds. Researchers therefore strive to develop a reliable toxicity prediction model enabling high throughput screening in an effort to catch up with this swift pace of new chemicals. The quantitative structure-activity relationship (QSAR) models, which is based on the hypothesis that chemicals with similar molecular structures can show similar biological activities, are currently considered as an *in silico* alternative to bioassays for statistically estimating toxicity. However, this semi-empirical approach also suffers from anti-examples of chemicals with similar molecular structure but exhibiting different biological activity. This reflects that there is a more profound mechanism of chemical toxicity involving not only geometric structure of a molecule but also its electronic structure-related properties.

In this talk, I will review current in silico approaches to the toxicity assessment such as QSAR and molecular docking models and their performance to evaluate adverse effect of polycyclic aromatic hydrocarbon molecules with respect to in vitro assays. An approach based on the first principles calculation will be also proposed as a new bio-physical communication model predicting reaction between chemical substance and AhR receptor.

***Coffee and Cookies will be served in Physics lounge at 3:00 p.m. for those attending the seminar.***