The Iby and Aladar Fleischman
Faculty of Engineering
Department of Materials Science and Engineering

אוניברסיטת תל-אביב
TEL AVIV UNIVERSITY

הפקולטה להנדסה
ע"ש איבי ואלדר פליישמן
המחלקה למדע והנדסה של חומרים

You are cordially invited to attend this seminar to be held on

## Tuesday, April 28th, 12:00
## Room 206, Wolfson Mechanical Engineering Building

# Atomic Scale Simulation in the Service of Nuclear Materials

## Prof. Robin Grimes
Chief Scientific Advisor, Foreign and Commonwealth Office, UK Government
Professor of Materials, Imperial College, London

In the presence of His Excellency Matthew Gould, British Ambassador to Israel

Our understanding of materials performance is based on experimental data. We use it to generate predictive models that allow us to develop improved materials and sometimes even select new materials or compositions. With nuclear energy related technologies, however, experimental data is often difficult to obtain either because the controlling factor takes place on time scales or length scales such that facilities are not available or the hazard is too challenging. In these circumstances atomic scale computer simulations can be exceptionally useful.

We can use the results of simulation in four different ways. First, most simply, to provide property values for existing models and add context to experimental data such as the extent of defect volumes changes associated with fission product lattice defects. Second, to 'check' or 'test' existing assumptions – as we have for the potential burnable poison $ZrB_2$. Third, to improve existing models by 'developing' the physical models – as with our understanding of the role that additives have on improving the durability of nuclear waste glass. Sometimes, however, it is possible to develop totally new models so the fourth approach uses simulations to 'discover' or 'identify' the physics/chemistry behind the process – here we will consider dislocation processes in $UO_2$.

Thus, we will consider these four issues in turn to illustrate how modelling and simulation adds value to the development of nuclear materials.

## Biosketch

Robin Grimes is the UK Foreign and Commonwealth Office Chief Scientific Advisor. He is also Professor of Materials Physics at Imperial College and was previously Director of the Imperial College Centre for Nuclear Engineering and the Rolls Royce University Technology Centre in Nuclear Engineering. His primary research interest is the application and development of computer simulation techniques to predict structural and dynamic properties of inorganic materials for energy applications. He has published over 270 scientific papers.