

先进计算与数字工程学术讲座

Title: Beyond Structure - Multiscale Modeling of Chemical and Biophysical Processes in Complex Environments

报告人: Dennis Salahub 教授

(加拿大卡尔加里大学)

主持人:魏彦杰研究员

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ABSTRACT

The report will progress on some of the following applications in the areas of biomolecular modeling, nano-catalysis for oil sands upgrading, and earth science – humic and fulvic substances.

- 1. Biomolecular modeling
- 2. Nano-catalysis for oil sands upgrading
- 3. Humic and fulvic substances

BIOGRAPHY

诚挚邀请全院感兴趣的同事同学参加!

Dennis Salahub is a Professor of Chemistry at the University of Calgary. He is also affiliated with the Centre for Molecular Simulation, the Institute for Quantum Information Science and with Quantum Alberta. Dr Salahub's interests are in the field of theoretical and computational chemistry, especially in the theory and applications of Density Functional Theory. He has published over 325 research papers and four edited books, and has delivered more than 475 invited lectures nationally and internationally. His publications have been cited some 19 000 times and his h-index is 66. The deMon software that originated in his laboratory is used by hundreds of researchers around the world.

Enquiries: Ms. Luo. Tel:86392309 E-mail: pd.luo@siat.ac.cn