



“固体所青联会”第五十七期

# 学术论坛

**题目：** Applications of multiscale computational nanoscience towards sustainable energy

**报告人：** Prof. Miranda (巴西圣保罗大学)

**时间：** 2017年2月22日 (周三) 上午 09: 30

**地点：** 固体所新楼520会议室

**报告内容简介：** In this talk, Prof. Miranda will summarize some new findings based on multiscale molecular simulations to search for i) nanostructured based materials for ethanol catalysis, ii) a first-principles characterization for thermoelectric applications (hosting trivalent guest ions in type-I Ge clathrates) and iii) displace more oil by controlling the chemical environment of oil/brine/rock interfaces using functionalized nanoparticles or nanoporous media.

**报告人简介：** Caetano R. Miranda, Professor in the Institute of Physics in the University of São Paulo (USP). He has experience in Condensed Matter Physics and Materials Science, working mainly in the area of Computer Simulation of Materials, applied to energy and environmental issues: renewable energy (hydrogen, fuel cells and batteries for solar fuels), Nanotechnology for the oil industry and construction materials, techniques Computational Physics and Materials under extreme conditions.

