# 数学与系统科学研究院

# 计算数学所网络学术报告


## 报告人：Prof. Shaoqing Wang

（ *Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences* ）


## 报告题目：

## Numerical Molecular Vibration

## 邀请人：　曹礼群 研究员

## 报告时间：2020 年 12 月 10 日（周四）

## 下午 14:00-15:00

## 报告工具：腾讯会议（ID：694 742 903）

会议链接：

**https://meeting.tencent.com/s/QnopZPflYHgR**

# 摘要：

**It is essential to clarify the intrinsic molecular vibration behavior in order to understand the structure, various physical and chemical properties of the molecule. In this talk, I will introduce two efficient methods, the Eckart frame algorithm and the multiorder derivative algorithm [1], for vibrational frequency calculation directly based on the raw data of atomic trajectory from the state-of-the-art first-principles molecular dynamics simulation. Vibrational assignment establishes the correspondence between vibrational modes and spectral frequencies. The unambiguous assignment for each of the calculated fundamental frequency by the frequency-domain filtering algorithm is realized. These rigorous numerical algorithms have been used to solve some historical issues on the molecular vibration of benzene [2]. As a major achievement, the experimental frequencies of benzene a2g and b2u vibrations are reassigned, which breaks a deadlock in contemporary spectroscopic science and removes a cloud over the application of density-functional theory in organic chemistry. Our work paves the way for the comprehensive realization of the first-principles spectroscopic research, and provides crucial clues to solve the century-old problems of Kekule resonance, p-deformation, and aromaticity.**

# 个人简介：

王绍青：博士生导师，沈阳材料科学国家研究中心首席研究员(PI)、中国科学院知识创新工程课题组长、沈阳市领军人才。中国计算物理学会理事会理事、中国材料学会计算材料学分会委员。曾留学访问英国剑桥大学、美国麻省理工学院、德国亚琛工业大学、俄罗斯列别捷夫物理研究所等国际学术机构。主持完成三项科技部 973 项目课题和七项国家自然科学基金委项目，荣获国家和省部级科学技术奖三项。**Webpage: https://publons.com/researcher/1313205/s-q-wang/**

# 欢迎大家参加！