

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. Zhijian Yang**

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报告题目:

Atomistic-based stress evaluation

邀请人: 许现民 副研究员

报告时间: **2020 年 10 月 19 日(周一)**

下午 16:00-17:00

报告工具: **腾讯会议 (ID: 631 751 090)**

会议链接:

<https://meeting.tencent.com/s/JmvJNSfshXlx>

Abstract:

Constitutive relation is one of the most important properties of materials. Either experiments or massive MD/MC simulations are needed to get such material properties. In this talk, I will discuss different aspects of atomistic-based stress definition and evaluation. I will discuss the definition of stress at atomistic level for small systems, which is consistent with conservation laws at macroscopic level. I will also talk about effective and practical algorithms to evaluate stresses for both homogeneous and inhomogeneous systems, with or without temperature effects, with or without defects. Some theoretical results will also be provided.

欢迎大家参加！