

数学与系统科学研究院

计算数学所学术报告

报告人： 罗晓光 副研究员

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报告题目：

**Searching Non-ablative Thermal
Protection Materials: from Materials
Design to Preparation**

邀请人： 曹礼群 研究员

报告时间： 2017 年 4 月 28 日 (周五)

上午 10:30-11:50

报告地点： 数学院南楼七层

714 教室

Abstract:

Some classic materials designs methodology as the first-principles (ab initio), molecular dynamics, computational thermodynamics is attempted in searching new kinds of materials which are used as non-ablative thermal protection materials for hypersonic space vehicles. To predict the high temperature properties of condensed matter, the quasi-harmonic approximation (QHA) is embedded in the first-principles calculations. Solids typical thermodynamic and finite-temperature static elasticity is calculated to validate the QHA model. Furthermore, a set of classic atomic potentials, with a Tersoff potential function type, are developed to use in molecular dynamics simulations.

欢迎大家参加！