

Joint CQSE and CASTS Seminar

Weekly Seminar
Oct. 7, 2016 (Friday)

TIME Oct. 7, 2016, 14:30 ~ 15:30
TITLE Ab initio study of energetic materials under pressure
SPEAKER Dr. Kunchala Ramesh Babu
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PLACE Rm716, CCMS & New Physics Building, NTU

Abstract

Solid energetic materials play an important role as explosives and fuels. Inorganic azides, a class of energetic systems, are potential model systems to study fast reactions in chemically complex solids that undergo deflagration or detonation. Some of the metal azide systems used as parent compounds to obtain polymeric nitrogen, an ultimate green high energy material. Most of the inorganic azides show variation in stability towards heat, light, and shock. To understand the decomposition phenomena, knowledge of electronic band structure and optical properties are essential. In this talk, we will present the results of density functional calculations on crystalline alkali metal azide systems. As these compounds are molecular solids, we also include the semi-empirical vander Waals interactions (vdW) in our calculations for the complete description of the crystal structures. The high pressure structural behavior of LiN_3 , KN_3 and RbN_3 will be discussed. In particular, the effect of pressure on electronic, optical and vibrational properties of the systems will be presented.

