武汉物数所理论交叉学术交流系列报告 (第一八六期)

Tale of A Novel Energetic Material of TKX-50



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Abstract: Our insight into the physicochemical properties of TKX-50, a novel energetic material with excellent performance, will be provided in my report. It contains: (1) It exists three phases for TKX-50. (2) The unusual Protonation of HA+ is responsible for the relatively low thermal stability of TKX-50. (3) Reversibility of the proton transfer in TKX-50 severs as an absolutely new mechanism for low impact sensitivity. (4) That the two-sided effects of strong hydrogen bonding on the Stability of TKX-50 set a base for designing new EMs with respect to HBs. (5) The repulsion among H+ results in the enhancement of the thermal stability of TKX-50 by pressure increasing, which much differs from that the thermal decay becomes readier and readier through bimolecular reactions for common EMs like TNT when pressure increases.

报告人简介:中国工程物理研究院(中物院)化工材料研究所研究员,博士生导师。复旦大学物理化学博士毕业。中国化学会燃烧化学专业委员会成员,中国材料研究学会极端条件材料与器件分会成员,国防科工局专家组成员,中物院科学技术委员会材料与化学专业组成员,北京计算科学研究中心客座研究员,重庆大学、西南科技大学兼职研究生导师。《含能材料》编委。发起并主办全国性的学术会议"计算含能材料学论坛"和"中物院计算材料学与计算化学论坛"。承担国家自然科学基金和各类预研等课题共30余项。在JACS、JPCA/B/C、PCCP、CGD、CEC、JCC等期刊上发表论文100余篇。获"于敏数理奖"、"邓稼先青年科技奖"和"中物院科技创新一等奖"。

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