## Structural Arrangements of Nitromethane on the Graphene Surface

**LIU Ying-zhe, LAI Wei-peng, WANG Yu, YU Tao, REN Gan, GE Zhong-xue, KANG Ying**
(*State Key Laboratory of Fluorine & Nitrogen Chemicals, Xi'an Modern Chemistry Research Institute, Xi'an* 710065, *China*)

**Abstract**: Molecular dynamics simulations were performed to explore structural arrangements of nitromethane (NM) on the graphene (GRA) surface. The simulation results show that ordered and layered structural arrangements of NM are induced by the GRA surface. In the nearest layer to the GRA surface, the structural ordering is highest. The preferred orientation of NM is found, i.e. the dipole vector is parallel with the GRA surface, leading to more concentrated and higher density than bulk NM. To maximize the interactions between NM and GRA, furthermore, some NM molecules change from eclipsed structure to staggered structure. The influence of GRA on structural arrangements of NM is weakened as the distance between NM and GRA surface increases. The structural arrangements of NM trends toward disordered state of bulk NM started with the third layer.

**Key words**: density distribution; dipole orientation; ordering; molecular dynamics simulation
**CLC number**: TJ55; O64 **Document code**: A **DOI**: 10.11943/j.issn.1006-9941.2016.07.003

读者·作者·编者

## 《含能材料》“观点”征稿

为了丰富学术交流形式,及时传递含能材料领域同行们的学术观点和思想,《含能材料》开设了“观点”栏目。“观点”栏目的来稿应观点鲜明、内容新颖、形式上短小精悍。欢迎含能材料各领域的专家积极来稿。来稿时请附个人简介及主要研究工作介绍。

## 《含能材料》损伤与点火专栏征稿

含能材料的损伤特征与点火过程有密切的联系,炸药、推进剂的内部损伤及其对力学特性、安全特性和点火行为的影响规律受到了含能材料学界的高度重视,为推动这一重要研究方向的学术交流,本刊特设立“损伤与点火”专栏。专栏主要征集炸药、推进剂等含能材料的损伤观测与多尺度表征技术、含损伤的本构方程、准静态与动态损伤演化规律、损伤与破坏的宏(细)观模式、损伤对起爆、爆炸、爆轰成长以及非冲击起爆行为的影响等方向的原创性研究论文。来稿请注明“损伤与点火”专栏。

《含能材料》编辑部