

CP2K

# BOMD, CP2K and Me



Trapping Gaseous  
Pollutants on  
Defective  
Graphene Sheet



UNIVERSITY OF  
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Line Defects at the  
Heterojunction of  
Hybrid Boron  
Nitride/Graphene  
Nanoribbons

Selective trapping  
Increased trapping capacity

Dibyajyoti Ghosh

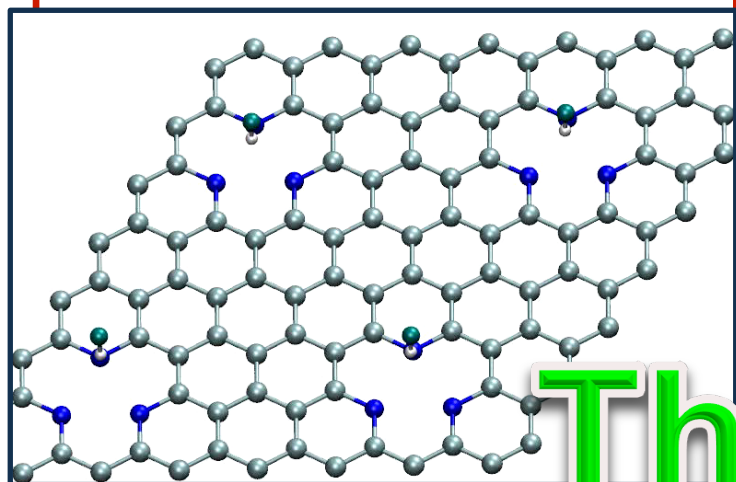
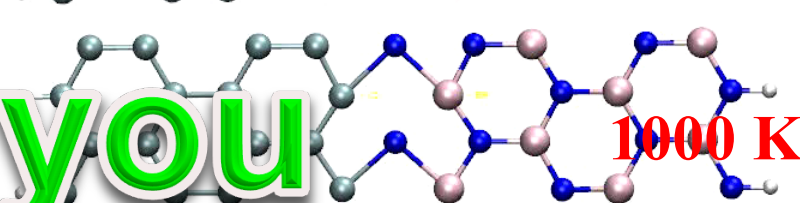
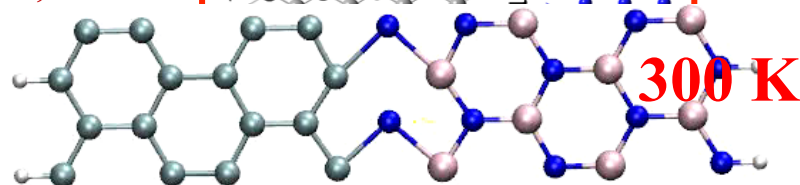
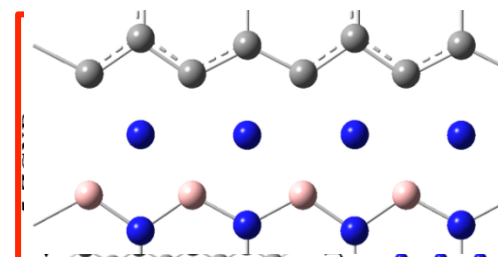
J. Mater. Chem.  
C, 2014, 2, 392

J. Phys. Chem.  
118, 1

Phys. Chem. C, 2013, 1

21700

vs. 2



Thank you