

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Effect of intercalated molecules on graphene sensing behavior

TAO SUN, KYOUNGMIN MIN, NARAYANA ALURU, Univ of Illinois - Urbana, COMPUTATIONAL MULTISCALE NANO SYSTEM TEAM¹ — The physical mechanism of graphene humidity sensor based upon capacitance measurement is explored by atomic/ab-initio simulations. Our simulations show that molecules intercalated between graphene and substrate (HfO₂) can have large influence on graphene sensing behavior. We find that oxygen vacancies on the surface of the substrate can induce an N-type doping in graphene, while oxygen molecules entering between the substrate and graphene will fill the vacancies and eliminate the N-type doping effect. We also observe that water molecules trapped at the interfacial layer can change the interlayer distance, thus changing the measured capacitance. Our simulations uncover the effect of intercalated molecules, which is helpful to better understand the operation process of graphene sensing devices.

¹Lead by Professor N R Aluru, we do multiscale simulations to explore mechanical and electronic properties of materials.

Tao Sun
Univ of Illinois - Urbana

Date submitted: 13 Nov 2014

Electronic form version 1.4