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Ultrasensitive Molecular Sensor Using N-doped Graphene through Enhanced Raman Scattering SIMIN FENG, Penn State University, MARIA CRISTINA DOS SANTOS, Universidade de Sao Paulo, BRUNO R. CARVALHO, Penn State University, RUITAO LV, Tsinghua University, KAZUNORI FUJISAWA, ANA LAURA ELIAS, MAURICIO TERRONES, Penn State University — As a novel and efficient surface analysis technique, graphene enhanced Raman scattering (GERS) has attracted increasing research attention in recent years. In particular, chemically doped graphene demonstrates much enhanced GERS effects than pristine graphene (PG) and it can be used to efficiently detect trace amount of molecules. However, the GERS mechanism is still an open question. Here, we present a comprehensive study on the GERS effect of PG and nitrogen-doped graphene (NG). By controlling the N-doping in NG, the Fermi level of graphene shifts, and if this shift aligns with the lower unoccupied molecular orbital (LUMO) of a molecule, charge transfer is enhanced, thus significantly amplifying the molecule vibrational Raman modes. We confirmed these findings using different organic fluorescent molecules. Interestingly, Raman signals from these dye molecules can be detected even for concentrations as low as 10^{-11}mol/L, thus providing excellent molecular sensing capabilities. In order to explain our results, these NG-molecule systems were modeled using dispersion corrected density functional theory. Furthermore, we demonstrated that when using different laser excitations, it is possible to determine the gaps between the HOMO and LUMO of different molecules.

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