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Experimental and theoretical investigations on SERS enhancement mechanism of graphene QINGZHEN HAO, Physics Department, SETH MORTON, Chemistry Department, BEI WANG, Physics Department, YANHUI ZHAO, Engineering Science and Mechanics Department, LASSE JENSEN, Chemistry Department, TONY JUN HUANG, Engineering Science and Mechanics Department, The Pennsylvania State University — Graphene has recently been shown to improve the Surface-enhanced Raman Scattering (SERS) performance of traditional nanostructured metallic substrates. Here we present an experimental and theoretical study on its SERS enhancement mechanism. We observed that SERS enhancement of graphene can be tuned by changing its Fermi level via doping. Both molecular doping and gate doping experiments show that hole-doped graphene yields a larger SERS enhancement in methylene blue (MB) than electron-doped one. The MB-graphene system is then modeled using both a fully quantum mechanical (QM) description as well as a QM-polarizable force field model wherein the graphene is modeled using a Drude-Lorentz function. In the first model, charge transfer (CT) excitations between MB and a graphene cluster can be accounted for, while in the second model we can account for the "infinite" size of the graphene sheet. Both of the models confirm the role of graphene Fermi level on its SERS enhancement. Our preliminary results suggest that graphene SERS enhancement would likely be coming from a ground-state chemical enhancement.

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