

Abstract Submitted  
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**Fluctuation effects of local electric field induced by water on graphene dot band gap**<sup>1</sup> SERGIO DALOSTO, SILVIA TINTE, INTEC, Univ. Nac. Litoral, Santa Fe, Argentina — Graphene, a two-dimensional single plane of carbon atoms, has shown to have favorable chemical sensor properties. In particular, ubiquitous molecules such as water could affect the sensitivity and selectivity of graphene. We investigate the fluctuations in the HOMO-LUMO gap of graphene dots due to the interaction with water using a combination of first principles and molecular mechanics (QM/MM) and classical molecular dynamics (MD). Our major conclusion is that the HOMO-LUMO gap for both spin flavors fluctuates following the variation of the local electric field at both zigzag and armchair edges. The local electric field is not uniform at the edges along the MD simulations. These results may be useful in the design of sensors based on graphene.

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