Chemically tunable transport phenomena of functionalized graphene

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We present an *ab initio* multiscale study and quantum transport simulations using the Kubo formalism [1] of chemically modified graphene based materials, whose properties are tuned by changing the density and nature of grafted molecular units. Depending on the nature of the introduced molecular bonding different conduction mechanism are obtained, including transition from weak to strong Anderson localization [2,3], as well as spin-dependent phenomena[4]. Experimental results[5] supporting the interpretation as a metal-insulator in the case of ozone treatment are also provided.

References

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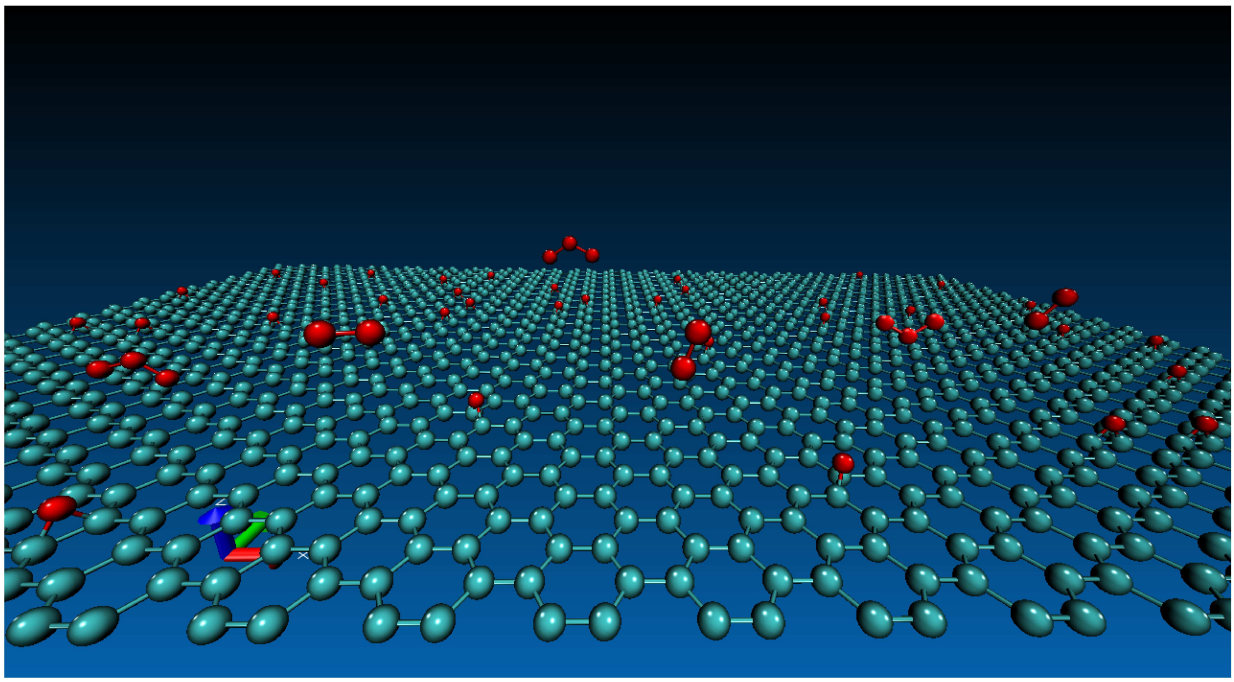
Figures



Functionalization of graphene due to ozone treatment