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Electronic Properties of Graphene: Insights from Atomistic Calculations

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First principles calculations have become useful tools to understand, predict and model the physical properties of material systems. Their predictive capabilities combined with the continuously growing computational power have turned them into computational microscopes invigorating the dialogue between theory and experiment. In this talk I will show how these calculations can be used to study the electronic properties of graphene such as charge screening and contact resistance [1-3]. Owing to its outstanding physical properties this two-dimensional material system has attracted lot of attention not only for basic science but also technological applications.

[1] M.A. Kuroda et al., "Conductance through Multilayer Graphene Films," Nano Lett. **11**, 3629 (2011).
[2] M.A. Kuroda et al., "Nonlinear Screening in Multilayer Graphene Systems," Phys. Rev. Lett. **106**, 116804 (2011).
[3] M.A. Kuroda et al., "Optimal Thickness for Charge Transfer in Multilayer Graphene Electrodes," Phys. Rev. Appl. **1**, 14005 (2014).