Abstract Submitted
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First-principles simulations of doping-dependent mesoscale screening of adatoms in graphene[1] ARASH MOSTOFI, FABIANO CORSETTI, Departments of Materials and Physics, Imperial College London, DILLON WONG, Department of Physics, University of California, Berkeley, MICHAEL CROMMIE, Department of Physics, University of California, Berkeley, and Materials Sciences Division, Lawrence Berkeley National Laboratory, JOHANNES LISCHNER, Department of Materials, Imperial College London — Adsorbed atoms and molecules play an important role in controlling and tuning the functional properties of 2D materials. Understanding and predicting this phenomenon from theory is challenging because of the need to capture both the local chemistry of the adsorbate-substrate interaction and its complex interplay with the long-range screening response of the substrate. To address this challenge, we have developed a first-principles multi-scale approach that combines linear-scaling density-functional theory, continuum screening theory and large-scale tight-binding simulations. Focussing on the case of a calcium adatom on graphene, we draw comparison between the effect of (i) non-linearity, (ii) intraband and interband transitions, and (iii) the exchange-correlation potential, thus providing insight into the relative importance of these different factors on the screening response. We also determine the charge transfer from the adatom to the graphene substrate (the key parameter used in continuum screening models), showing it to be significantly larger than previous estimates.

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