

Abstract Submitted
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Anomalous magnetism in hydrogenated graphene NOEL GARCIA, JOSE LADO, JOAQUIN FERNANDEZ-ROSSIER, International Iberian Nanotechnology Laboratory (INL) — We revisit the problem of the local moment formation due to the functionalization of graphene by an individual chemisorbed Hydrogen atom. We first study the average spin magnetization as a function of the applied field, and we find that in the non-interacting case at $T = 0$, the $m_s(H)$ curve is non-linear for small H (at $T = 0$) which makes it impossible to define a spin susceptibility. Second, we compute the net magnetic moment within the mean field Hubbard approximation. In contrast with all previous work that use finite simulation cells that give a magnetic moment of $S = 1/2$, we use an embedding method that allows the modeling of a single impurity in infinite pristine graphene. Our results give a magnetic moment smaller than $1/2$. Our results highlight that the spin physics of a single Hydrogen is different from localized spin moments in gapped systems for which magnetic moment is quantized and from conductors, for which the $T = 0$ spin susceptibility do exist.

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