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First principles study of Stage-1 graphene intercalates, IBr and ICl[1] PRIYAMVADA JADAUN, LEONARD F. REGISTER, SANJAY K. BANERJEE, The University of Texas at Austin — In this study we examine, from a first-principles approach, the properties of 2 graphene intercalant systems namely, iodine monochloride (ICl-GIC) and iodine monobromide (IBr-GIC). These materials are being explored as possible interlayer dielectric candidates for 2D-to 2D-tunnel FETs (TFETs) and Bilayer pseudospin FETs (BiSFETs). To do so we employ density functional theory (DFT). Both these intercalants are stage-1 and acceptor type. We first put forth a structural description of these compounds that intercalate 2 successive layers of graphene, stacked AA type as obtained upon relaxation. Subsequently we describe the electronic structure of ICl-GIC and IBr-GIC and use it to predict the device suitability of these intercalants. It is seen that adding a layer of these GIC's to a single layer of graphene does not disturb graphene electronic spectra except for opening a small gap and introducing doping. With the second graphene layer added, coupling between the graphene layers becomes evident through a small amount of band splitting.

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