

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

GW Investigation of Alkali Intercalated Graphite BAHADIR ALTINTAS, Abant Izzet Baysal University, Department of Computer Education and Instructional Technology, RESUL ERYIGIT, Abant Izzet Baysal University, Department of Physics — The amount of charge transferred from the alkali atoms to graphene layers and the character of electronic energy levels have been controversial for the alkali intercalated graphite. Experimental studies by different techniques indicate negligible to full charge transfer, while DFT level calculations show a low level of charge transfer. We will report first principles calculations on electronic properties, such as charge transfer, band structure and partial density of electronic states of Li, Na, K, Rb and Cs intercalated graphite at the GW level. The results show a systematic increase in charge transfer compared to the DFT results as well as a raising of alkali derived states around the Fermi level

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Date submitted: 20 Nov 2009

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