

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

**Graphene oxide as a candidate material for natural gas storage:
A first principles study**¹ RAJIV KUMAR CHOUHAN, KANCHAN ULMAN,
TSU, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur, Banga-
lore, India, SHOBHANA NARASIMHAN, TSU, and Sheikh Saqr Laboratory, ICMS,
Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur, Bangalore, In-
dia — Alternative sources of clean energy will be much in demand in the coming
days. To store methane (CH_4) in sorbent materials at ambient conditions for on-
board vehicular usage, minimum adsorption energy of 18.8 KJ/mol is desirable. In
this work, we have investigated methane adsorption on graphene oxide using first
principles calculations. To accurately capture the weak interactions between CH_4
and the substrate we have included van der Waals interactions in our calculations.
We show that the adsorption energy falls within the target range. Careful analysis
of the various contributions to the binding shows that the enhancement in adsorp-
tion energy on going from graphene to graphene oxide arises from a subtle synergy
between various effects.

¹Funding agencies CSIR, India, DST Nanomission and JNCASR. Computational
facilities provided by TUE-CMS, JNCASR.

Rajiv Kumar Chouhan
Boise State University, Boise, ID

Date submitted: 15 Nov 2014

Electronic form version 1.4