Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Ab Initio Calculations of Nitrogen Functionalization of Graphene OLIVIER MALENFANT-THUOT, GERMAIN ROBERT-BIGRAS, LUC STAFFORD, MICHEL CÔTÉ, Université de Montréal — Our collaboration between theorists and experimentalists aims to achieve nitrogen functionalization of graphene with the late-afterglow regime of a microwave plasma. We hope this technique will give us a better control on the functionalization due to the small density of interacting atoms in the late-afterglow and a drastic diminution of induced defects compared to standard plasma functionalization techniques. With the software package ABINIT, we carried out first-principles calculations of different nitrogen atoms configurations in a graphene sheet. We obtained their formation energies to study whether they are realistic. We found that vacancies in the graphene sheet facilitate the incorporation of nitrogen atoms and, in particular, that the substitutional doping has the lowest formation energy. We also studied the energetic of nitrogen atoms adsorbed above the carbon plane and the interactions between those atoms. Using the Nudged Elastic Band method (NEB), we were able to calculate energy barriers for the diffusion and the in-plane absorption of these atoms.

Olivier Malenfant-Thuot
Université de Montréal

Date submitted: 10 Nov 2016 Electronic form version 1.4