Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

First principle studies of doping effects on the electronic and geometric structures of graphitic C3N4 SEBASTIAN ZULUAGA, SERGEY STOLBOV, University of Central Florida — Layered carbon nitride g-C3N4 is a promising material as a photo-anode for the H production from water. By doping, the band gap (2.7 eV) can be tuned to the value optimal for efficient absorption of visible light irradiation. We present here our first principle computational study of the effects of doping with B, P and S on the geometric and electronic structures of g-C3N4 and compare them to experimental results. We have evaluated within density functional theory the energetics of various doping scenarios in terms of both thermodynamics and kinetics, and selected the energetically most favorable structures. Our calculations reveal important details of valence charge density redistribution upon the doping. The doping effect on the electronic density of states (DOS), in particular on band gap width, has been evaluated using an accurate GW method. We find the DOS to strongly depend on the doping geometry. The detailed analysis of the projected DOS provides significant insight into the mechanism underlying modification of the electronic structure upon doping.

Sebastian Zuluaga
University of Central Florida

Date submitted: 11 Nov 2012 Electronic form version 1.4