

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Gas molecule adsorption on silicene nanoribbons: Conductance modulation and contact effects¹ TIM OSBORN, AMIR FARAJIAN, Mechanical and Materials Engineering: Wright State University — We investigate the effects of adsorption of gas molecules on the quantum conduction of silicene nanoribbons with and without silver contacts, using ab initio methods and Green's function formalism. The adsorption positions and orientations are determined through energy calculations and structure optimizations for NO₂, CO₂, and CO gas molecules. The conduction change upon gas molecules adsorption is studied for isolated silicene nanoribbons and for silicene nanoribbons on silver side contacts for potential applications as ultrasensitive nanoelectrochemical sensors.

¹This project is supported by the National Science Foundation grant ECCS-0925939.

Tim Osborn
Wright State University

Date submitted: 07 Dec 2010

Electronic form version 1.4