Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Binding sites and diffusion barriers of a Ga adatom on the GaAs(001)-$c(4 \times 4)$ surface from first-principles computations[1] J. ROEHL, A. KOLAGATLA, V.K.K. GANGURI, S. KHARE, University of Toledo, R.J. PHANEUF, University of Maryland — The Ga adatom adsorption and diffusion processes on the GaAs(001)-$c(4 \times 4)$ surface were studied using *ab initio* density-functional-theory computations in the local density approximation. Two distinct sets of minima and transition sites were discovered for a Ga adatom relaxing from heights of 3 and 0.5 Å from the surface. These two sets show significant differences in the interaction of the Ga adatom with surface As dimers. An electronic signature of the differences in this interaction was identified. We computed the energetic barriers to diffusion for various adsorption sites. From these, we propose three pathways for diffusion of a Ga adatom on this surface which indicate anisotropic diffusion along different directions.[2]

[1]J.L. Roehl *et al.*, Phys. Rev. B **82**, 165335 (2010).
[2]Supported by NSF DMR 0705464.

Jason Roehl
University of Toledo

Date submitted: 26 Nov 2010 Electronic form version 1.4