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SIESTA study of c-GaN(001)-4x1 surface reconstruction: Tetramers andtheir STM images. NANCY SANDLER, HAMAD AL-BRITHEN, MUHAMMAD HAIDER, ARTHUR SMITH, Ohio University, PABLO ORDEJON, Instituto de Ciencias de Materiales, Barcelona, Spain — Recent STM, STS and RHEED studies [1] on cubic GaN(001), grown using rf MBE under Ga-rich conditions, have revealed a surface structure consistent with predicted tetramer formation [2,3]. STM images reveal a surface consisting of rows aligned along the [110] direction with a periodicity along the [1$\underline{1}$0] direction of about 12.8$\mathring{A}$. STS measurements indicate the semiconducting nature of the surface and RHEED patterns of the surface provide further evidence of a periodicity consistent with tetramer formation. We report on a first principle study of this particular surface reconstruction using the SIESTA code [4], a self-consistent density functional method using standard norm-conserving pseudo-potentials and a flexible numerical linear combination of atomic orbitals basis set. Band structure calculations are in good agreement with previously reported results and the STM images obtained reproduce experimental observations. [1] H. Al-Brithen, M. Haider, A. Smith, N. Sandler and P. Ordejon. Submitted to PRL. [2] Neugebauer et al. Phys. Rev. Lett. 80, 3097 (1998) [3] Feuillet et al. Appl. Phys. Lett. 70, 24 (1997) [4] D. Sanchez-Portal, P. Ordejon, E. Artacho, and J. M. Soler, Int. Journ. of Quant. Chem. 65, 453 (1999).

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