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Ab initio investigation into the stability and electronic properties of GaN-nanowires D.J. CARTER, The University of Sydney, Australia, J.D. GALE, Curtin University of Technology, Australia, B. DELLEY, Paul Scherrer Institut, Switzerland, C. STAMPFL, The University of Sydney, Australia — Recent reports of successful fabrication of high quality gallium nanostructures such as quantum dots, nanocrystallites and nanowires, eg. [1], open the door to their possible role as important nanoscale building blocks for future optoelectronic, high-temperature/power and spintronic device applications. In the present work we perform *ab initio* calculations, using the DMol^3 [2] and SIESTA [3] codes, for wurtzite GaN nanowires. We have examined nanowires in the [0001], [10$\bar{1}$0], and [11$\bar{2}$0] directions, and investigated the stability, electronic and atomic structures as a function of nanowire radius. We found that only nanowires in the [0001] direction are stable, and that wires in the other directions can be stabilised by saturating dangling bonds with hydrogen. We have also investigated the properties of key point defects and dopants. [1] J. C. Johnson, *et al.* Nature Materials **1**, 106 (2002). [2] B. Delley, J. Chem. Phys. **92**, 508 (1990); *ibid* **113**, 7756 (2000). [3] J.M. Soler, *et al.* J. Phys.: Condens. Matter. **14**, 2745 (2002).

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