

Abstract Submitted
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Charge distribution on semiconductor nanorods PHILIP AVRAAM, PETER HAYNES, NICHOLAS HINE, PAUL TANGNEY, Imperial College, THOMAS YOUNG CENTRE TEAM — Semiconductor wurtzite nanostructures such as those of ZnO have been observed to exhibit a large dipole moment directed along the wurtzite polar-axis. Its presence can have implications for the optical properties of such nanostructures as well as for self-assembly. The surfaces on these nanostructures, particularly the polar (0001) surfaces, are thought to play a critical role in controlling the charge distribution. Reconstructions of polar surfaces in bulk crystals are known to be driven by the electrostatic requirement that the surfaces have neutral charge (resulting in a phenomenon called the “polar instability”), but those on wurtzite nanostructures do not have neutral charge, and little is known about the role played by surface polarity. We use the ONETEP code to perform linear-scaling plane-wave pseudopotential density-functional calculations on entire isolated GaAs nanorods consisting of thousands of atoms. We find novel relationships between the surface termination on both the lateral and polar surfaces and the charge distribution along the nanorod.

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