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Charge Distributions in Polar Semiconductor Nanorods explored with Linear-Scaling DFT Calculations NICHOLAS HINE, PHILIP AVRAAM, PAUL TANGNEY, PETER HAYNES, Thomas Young Centre, Imperial College London, United Kingdom — Binary polar semiconductors in the wurtzite structure can be grown as nanorods along ±[0001]. In such structures, large dipole moments have been observed. We have studied the distribution of charge in GaAs and ZnO nanorods to elucidate the origin of the dipole moments. To make contact with realistic experiments, rods containing thousands of atoms are simulated using Linear-Scaling DFT calculations with ONETEP [1]. From our calculations we show that both the direction and magnitude of the dipole moment of a nanorod, and its electric field, depend sensitively on how its surfaces are terminated, not on the spontaneous polarization of the underlying lattice. Furthermore, we observe that the Fermi level for an isolated nanorod always coincides with significant density of electronic surface states on its polar surfaces (either mid-gap states or band-edge states). These states pin the Fermi level, and therefore fix the potential difference along the rod. We provide evidence that this effect has a determining influence on the polarity of nanorods, with consequences for the response to changes in surface chemistry, scaling of dipole moment with size, and dependence of polarity on composition.

[1] C. Skylaris et al, JCP 122, 084119 (2005).
[2] P. Avraam et al, PRB 83 241402(R) (2011).

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