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Understanding polarity in semiconductor nanorods with linear-scaling density-functional theory simulations PETER HAYNES, PHILIP AVRAAM, Imperial College London, NICHOLAS HINE, University of Cambridge, PAUL TANGNEY, Imperial College London — Binary polar semiconductors with the wurtzite structure have been observed to exhibit large dipole moments along [0001]. To explore the origin of these dipole moments, we use a linear-scaling density-functional theory code [1] to perform first-principles calculations of entire wurtzite GaAs nanorods consisting of several thousand atoms. We find that both the direction and magnitude of the dipole moment of a nanorod, and the electric field, depend sensitively on how its surfaces are terminated and not strongly on the spontaneous polarization of the underlying lattice [2]. We show that our calculations can be explained in terms of a pinning of the Fermi level at the polar surfaces that fixes the potential difference across the nanorod, and that this effect can have a determining influence on the polarity of nanorods, with consequences for the way a nanorod responds to changes in its surface chemistry, the scaling of its dipole moment with its size, and the dependence of polarity on its composition [3]. We discuss the implications of these results for tuning nanocrystal properties, and for their growth and assembly.

[1] J. Chem. Phys. 122, 084119 (2005).
[2] Phys. Rev. B 83, 241402(R) (2011).
[3] Phys. Rev. B 85, 115404 (2012)

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