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**The dipole moments of ZnO nanorods** SEFA DAG, SHUZHI WANG, LIN-WANG WANG, Lawrence Berkeley National Laboratory — A self-consistent linear scaling three dimensional fragment (LS3DF) method is used to study the dielectric properties of large ZnO nanorods. Our ab initio calculations show that the ZnO nanorod with unpassivated (10-10) side surface has a large dipole moment which is caused by both surface and interior bulk dipoles. An systematic analysis is carried out, and we found that the biggest contribution to the total dipole moment is from the (10-10) surface. Dielectric screening model is used to illustrate how the dipole moment changes with nanostructure size and geometry. We also show the effect of the dipole moment on the interior electronic structure of the nanorod.

Sefa Dag  
Lawrence Berkeley National Laboratory

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