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The electronic structure of radial p-n junction silicon nanowires SHAN-HAW CHIOU, Industrial Research Technology Institute, JEFFREY GROSSMAN, U.C. Berkeley — Silicon nanowires with radial p-n junctions have recently been suggested for photovoltaic applications because incident light can be absorbed along the entire length of the wire, while photogenerated carriers only need to diffuse a maximum of one radius to reach the p-n junction. If the differential of the potential is larger than the binding energy of the electron-hole pair and has a range larger than the Bohr radius of electron-hole pair, then the charge separation mechanism will be similar to traditional silicon solar cells. However, in the small-diameter limit, where quantum confinement effects are prominent, both the exciton binding energy and the potential drop will increase, and the p-n junction itself may have a dramatically different character. We present ab initio calculations based on the generalized gradient approximation (GGA) of silicon nanowires with 2-3 nm diameter in the [111] growth direction. A radial p-n junction was formed by symmetrically doping boron and phosphorous at the same vertical level along the axis of the nanowire. The competition between the slope and character of the radial electronic potential and the exciton binding energy will presented in the context of a charge separation mechanism.

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