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Gate controlled donor activation in silicon nanowires ADAM GALI, Research Institute for Solid State Physics and Optics of the Hungarian Academy of Sciences, BINGHAI YAN, THOMAS FRAUENHEIM, Bremen University — Due to the proximity to an embedding medium with low dielectric constant (e.g., oxides), semiconductor nanowires have higher impurity ionization energy than their bulk counterparts, resulting lower free carrier density. Using ab initio calculations within density functional theory, we propose a way to reduce the ionization energy in nanowires by fabricating a special cross section with appropriate engineering of doping and an applied gate voltage. We demonstrate on a phosphorus-doped silicon nanowire that the ionization energy can be effectively tuned and the impurity backscattering can also be reduced. For instance, the free carrier density may increase by 40% in a silicon nanowire with 15 nm diameter and special cross section without special engineering of doping. Our proposal has profound implications to fabricate nanowire devices with high carrier density. Our proposed Si NW device realizes a fine manipulation of the interaction between electron and nuclear spins by using an external electric field which is a fundamental step to a silicon-based nuclear spin quantum computer. Moreover, with a negative voltage the ionization energy of P-donors can be increased even in larger silicon nanowires which opens up the possibility to manipulate the donor electron spin at room temperature [1]. [1] B. Yan, Th. Frauenheim and A. Gali, *Nano Lett.*, 2010, 10, 3791

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