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Origin of Giant Piezoresistance in Pristine <111>-Si nanowires¹ JUEXIAN CAO, RUQIAN WU — It was found recently that silicon nanowires possess an unusually large piezoresistive coefficient, 350 times higher compared with Si bulk. Using first principles density functional calculations, we demonstrated that this stems from the strain-induced change in band ordering of surface states. The pristine <111>-Si nanowire is metallic under ambient condition but the mobility of the carrier is extremely small due to the strong localization. The compression shrinks the surface shell and hence shifts the itinerant state across the Femi level, which consequently leads a surge in conductance. The effective masses of those two bands differ by a factor of 100, a number that can roughly account the experimental data. Since the key bands for transport are surface states, the surface modification plays a vital role on the piezoresistance effects, as observed experimentally.

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