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**Supplementary Material for:**  
**Influence of Surface Passivation on Indium Arsenide Nanowire  
Band Gap Energies**

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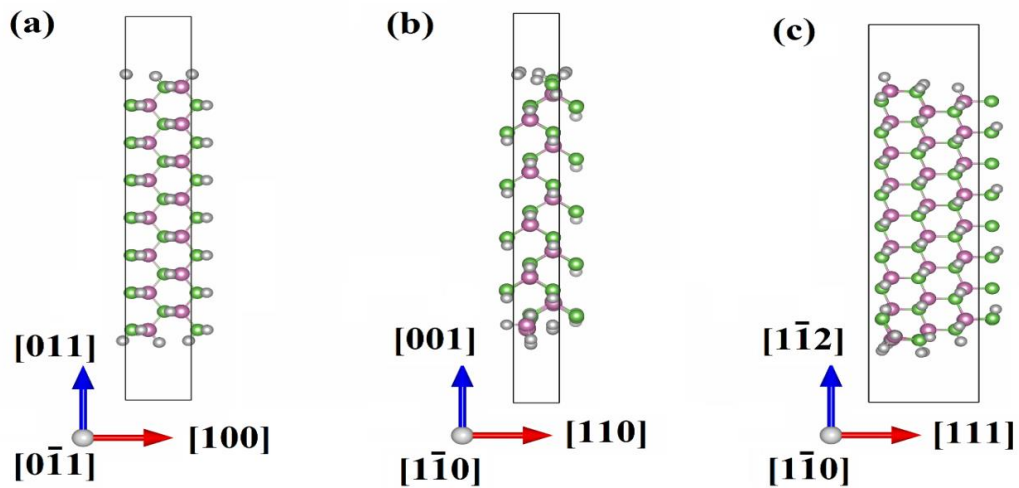


Figure S1. Side view of the structure of (a) [100]-oriented, (b) [110]-oriented, and (c) [111]-oriented InAs and GaAs nanowires used in this work. Green spheres are In/Ga, purple spheres are As, and grey spheres schematically indicate surface passivation for the terminating groups –pseudo-H, -H, -F, and -NH<sub>2</sub>. Images rendered using VESTA [33].

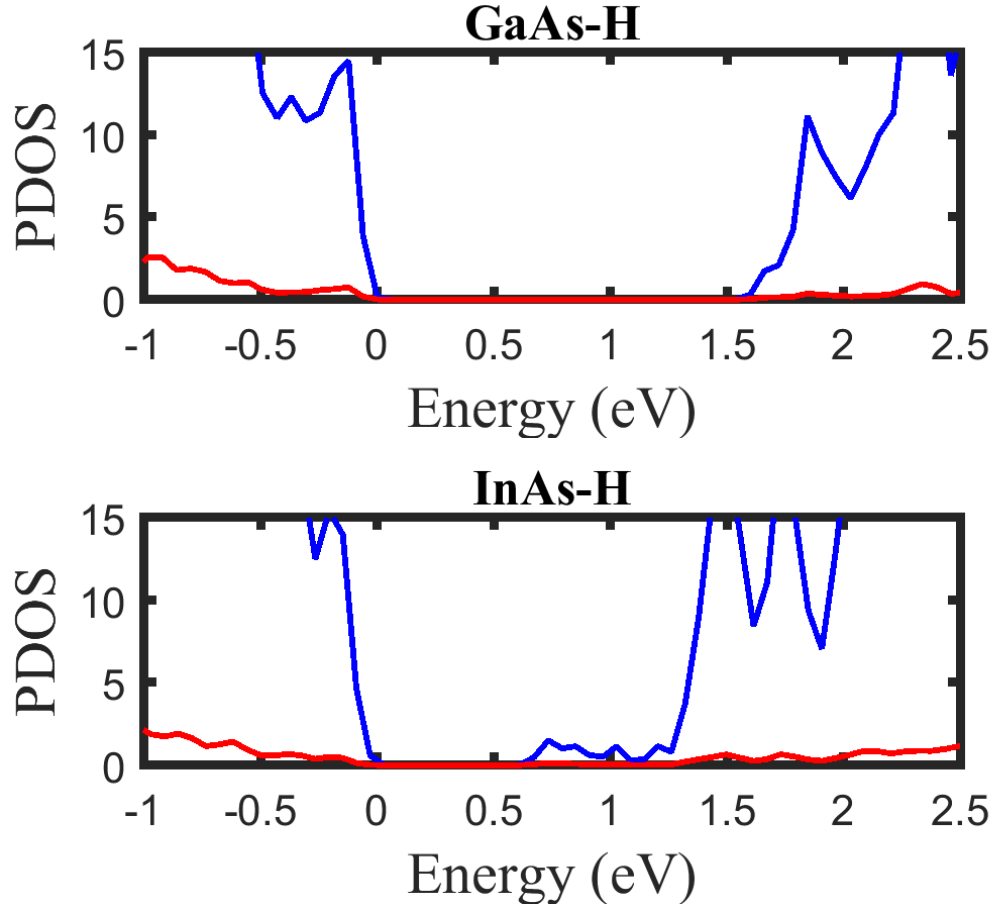


Figure S2. Projected density of states (PDOS) for the (a) 1.6 nm [100]-oriented GaAs NWs and (b) 2.0 nm [100]-oriented InAs NWs with -H surface terminations. The DoS of states is decomposed into contributions of core In-As nanowire (blue) and the surface passivating species (red). Energies are referenced with respect to the conduction band edge.

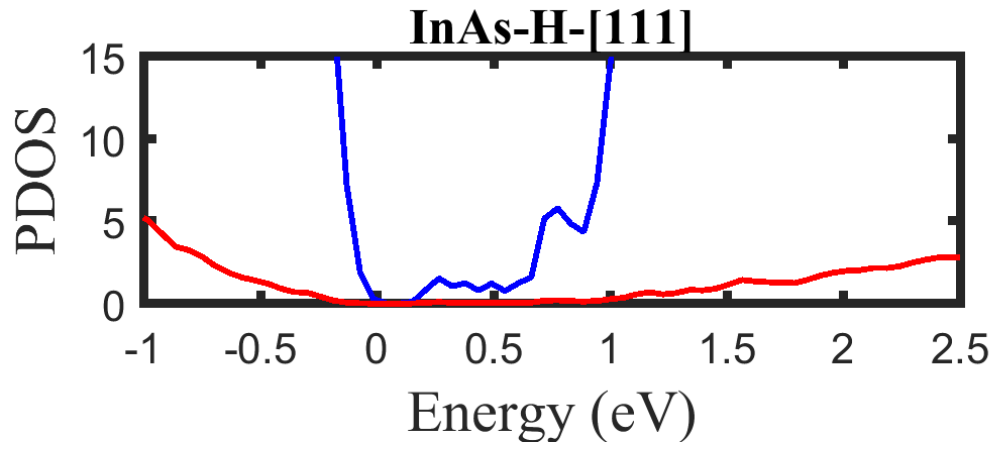


Figure S3. Projected density of states (PDOS) for the 3.0 nm [111]-oriented InAs NWs with -H surface terminations with the DoS decomposed into contributions of the core In-As nanowire (blue) and the surface passivating species (red). Energies are referenced with respect to the conduction band edge.