

## Supporting information:

# Shell Thickness Dependent Tunable Threshold Voltage Single Quantum Dot Rectification Diode

*Gopal Sankar Kenath<sup>‡</sup>, Rekha Mahadevu<sup>¶</sup>, Anand Sharma<sup>‡</sup>, Vinod K Gangwar,<sup>€</sup> Sandip  
Chatterjee,<sup>€</sup> Anshu Pandey<sup>¶</sup> and Bhola N. Pal<sup>‡\*</sup>*

<sup>‡</sup>School of Materials Science and Technology, <sup>€</sup>Department of Physics, Indian Institute of  
Technology (BHU), Varanasi 221005, India

<sup>¶</sup>Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore 560012, India

\*Corresponding Author: [bnpal.mst@itbhu.ac.in](mailto:bnpal.mst@itbhu.ac.in)

### Synthesis of ZnTe/CdS core/shell QDs:

Tellurium (Te, 99.99%), zinc chloride (ZnCl<sub>2</sub>, anhydrous 99.999%), sodium borohydride (NaBH<sub>4</sub> 96%), trioctylphosphine (TOP, technical grade, 90%), 1-octadecene (ODE, technical grade, 90%), oleylamine (technical grade, 70%), sulphur (S, <99.5%), and cadmium oxide (99.9%) were purchased from Sigma-Aldrich. 1,4-Butanediol (90%, AR) and dextrose (95% anhydrous, AR) were purchased from SD Fine Chemicals. All chemicals were used without further purification. Zinc Telluride (ZnTe) Nanoparticle Synthesis. This synthesis involves two steps: initial preparation of sodium hydrogen telluride followed by the synthesis of ZnTe. Flask 1 Tellurium powder (0.1 mMol, 12.76 mg) and sodium borohydride (NaBH<sub>4</sub> 0.1 Mmol, 9.45 mg)

was added to a 50 mL three-necked flask containing 1 mL of diol (i.e., 1,4-butanediol). This flask was heated at 60 °C under an argon atmosphere for about 15 minutes. NaBH<sub>4</sub> reduces elemental tellurium (Te(0)) to its Te(II) state. Dextrose (0.1 mM in 1 mL of 1,4-butanediol) was added to consume the excess borohydride. This step is important because the rapid injection of an unreacted borohydride solution into a heated flask (see step 2) may lead to a sudden release of hydrogen gas and an unexpected rise in pressure. TOP (0.2 mL) is then added (Flask 2) ZnCl<sub>2</sub> (0.1 mM, 13.63 mg) to a separate flask (flask 2) containing ODE (4 mL, from Aldrich) as solvent and oleylamine (1mL) as ligand. The mixture was degassed thoroughly and heated at 150 °C under an argon atmosphere. The contents of flask 1 were swiftly injected into flask 2. CdS Shell Growth on ZnTe Quantum Dots. We observed that elemental S dissolved in ODE can oxidize ZnTe NCs, and this precluded the straightforward use of S/ODE as the sulphur precursor. The sulfur precursor (SP) was prepared by heating 32 mg of S powder in 5 mL of oleylamine at 250 °C for 5 minutes under an argon atmosphere. The resultant reddish solution was diluted with 5 mL of ODE. The cadmium precursor (CP), cadmium oleate, was separately prepared by heating 128 mg of cadmium oxide in oleic acid (3 mL) and octadecene (7 mL) at 300 °C for 10 minutes under argon. The resultant colorless solution was then degassed under vacuum for 5 min at 100 °C.

To grow ZnTe/CdS core/shell NCs, as-prepared ZnTe NCs were heated at 250 °C. SP and CP were added drop wise alternately (2 mL of each per hour) until the desired shell thickness was achieved. CdS shells were grown on ZnTe cores by employing a more conventional approach, with a 0.1 M solution of sulfur in octadecene as the sulfur precursor and 0.1M cadmiumoleate as the cadmium precursor. The reaction was conducted at 220 °C under an argon atmosphere, with the ZnTe NCs dispersed in 4 mL of octadecene and 1 mL of oleylamine. The NCs were cleaned

thoroughly after synthesis, before proceeding to analysis and characterization. Care was taken to remove excess ligands, solvents, and unreacted precursors. Cleaning of NCs involved three steps. Initially, 5mL of methanol and 0.5 mL of ethanol were added to 5 mL of synthesized NCs, and the mixture was centrifuged for 1 minute at 900 RCF (relative centrifugal force). This led to the formation of two immiscible layers. The upper layer, which contained dissolved reaction by products and unreacted chemicals in ethanol, was separated from the lower layer, which contained NCs dissolved in octadecene.

The lower layer was used for the second step of purification. In the second step, 0.5 mL of methanol and 5mL of ethanol were added and kept for centrifugation for 1 minute at 900 RCF. For the third step, the lower layer was retrieved again, and 0.5 mL of methanol, 0.5 mL of ethanol, and 2 mL of isopropanol were added and kept for centrifugation for 1 minute at 900 RCF. The supernatant was removed, and the NCs were found precipitated in the form of a solid that adhered to the sides and the bottom of the tube. For device fabrication, the NCs were typically dissolved in octane with a concentration 5 mg/ml.