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A Novel Surface Modification Scheme for ITO Nanocrystals by Acetylene: A Combined Experimental and DFT Study

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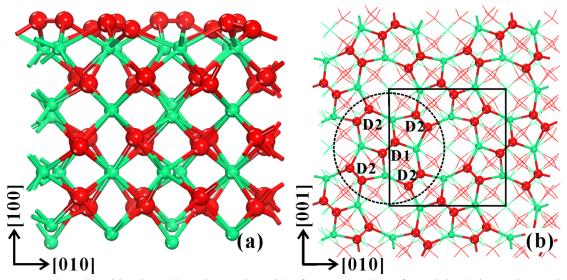


Figure S1. The side view (a) and top view (b) of In_2O_3 (100) surface slab. Color codes: red, O; green, In. The bond lengths of D1 and D2 are 1.475 and 1.506 Å, respectively.

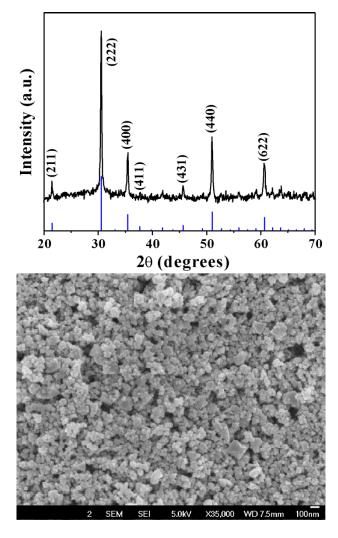


Figure S2. X-ray diffraction pattern and scanning electron microscopic image of ITO nanoparticles. Vertical blue lines show the standard pattern of body-centered cubic In_2O_3 (ICDD card no.: 06-0416).