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Electronic Supplementary Information

Strain Gradient Induced Spatial-Indirect Excitons in Single Crystalline ZnO Nanowires

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S1. Electronic Band Structures of Uniaxially Strained Bulk ZnO

Our calculations were performed with self-charge consistent density-functional tight-binding (SCC-DFTB) as implemented in dftb+ package. Bulk ZnO was strained along *c* axis. In structure relaxation, a *k*-point mesh of 15×15×15 within the Monkhorst-Pack special *k*-point scheme was chosen in the irreducible Brillouin zone. All atoms in the unit cell were allowed to relax by using the conjugate gradient energy minimization method until the force and charge on each atom reach their tolerance values of 10^{-6} eV Å^{-1} and 10^{-6} *e* respectively. The lattice parameters for relaxed strain-free bulk ZnO are $a_0 = 3.25$ Å, $c_0 = 5.20$ Å and $u = 0.38$. Figure S1 shows band structures of bulk ZnO under axial strain $\varepsilon = -1\%$, $\varepsilon = 0$, $\varepsilon = 1\%$ with *k* along *c* axis. The conduction band minimum (CBM) is contributed by Zn's 4*s* states and valence band maximum (VBM) is formed by hybridization of O's 2*p* and Zn's shallow 3*d* states. It is clear that CBM and VBM have the same shift direction when under strain. However, the energy shift of CBM is larger than that of VBM due to the remarkable $p - d$ coupling in ZnO.

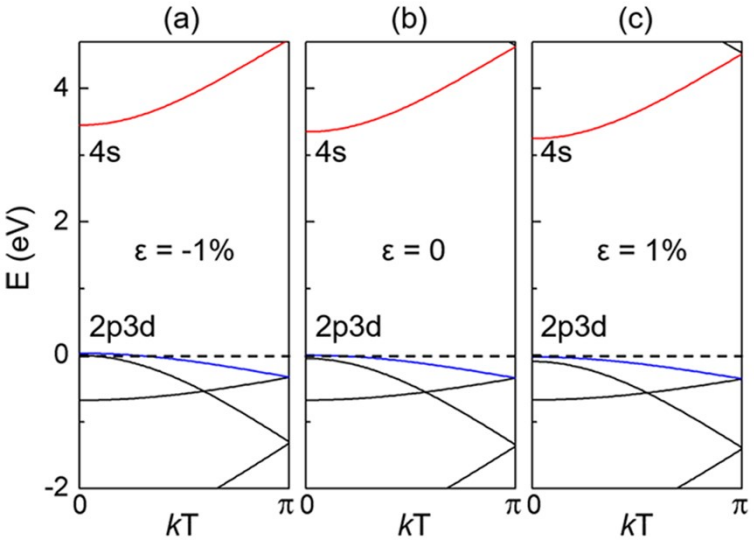

Fig. S1. Band structures of bulk ZnO under uniaxial strain along *c* axis. The band structures are obtained at strain (a) $\varepsilon = -1\%$, (b) $\varepsilon = 0$, and (c) $\varepsilon = 1\%$. Conduction band minimum (CBM) and

valence band maximum (VBM) are in red and blue colors respectively. Dashed line indicates the VBM of strain-free bulk ZnO.

S2. Spatial Charge Distributions of Conduction and Valence Band States for ZnO Nanowires with Small Bending Deformation

For the bent ZnO NW under bending angle $\Omega = 0.045^{\circ}$, Fig. S2(a) shows the charge density distributions of valence band minimum (VBM) state, VBM−1, VBM−2, and VBM−3 at $\kappa = 0$. Sum_{VB} at the rightmost of Fig. S2(a) is a sum of the charge density of these four states. Figure S2(b) shows the charge density distributions of conduction band maximum (CBM) state, CBM+1, CBM+2, and CBM+3 at $\kappa = 0$. Sum_{CB} at the rightmost of Fig. S2(b) is a sum of the charge density of these four states. The obtained charge distributions of Sum_{VB} and Sum_{CB} indicate that the indirect exciton picture is not valid at small bending angle.

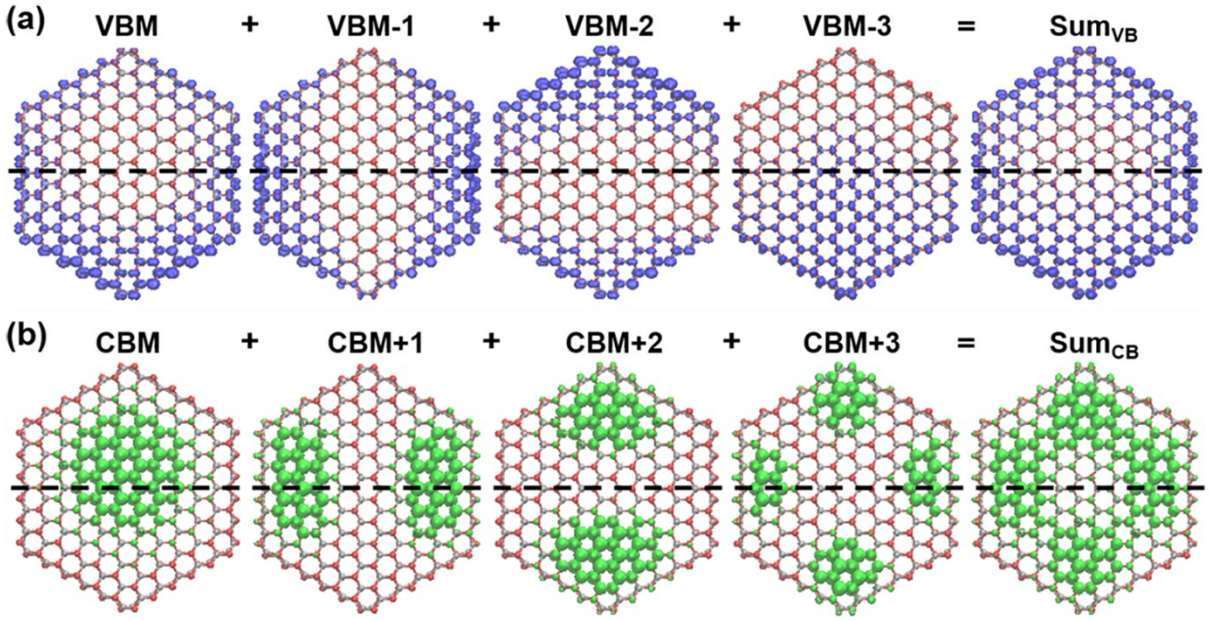

Fig. S2. Spatial charge distributions of conduction and valence bands at Γ point for ZnO nanowires (D = 3.63 nm) with bending angle $\Omega = 0.045^{\circ}$. The valence band (VB) and conduction band (CB)

states are in blue and green colors respectively. VBM−1, VBM−2, VBM−3 represent the first, second, third band below VBM and CBM+1, CBM+2, CBM+3 represent the first, second, third band above CBM. The isosurface value for each individual state (VBM, ..., VBM−3, CBM, ..., CBM+3) is about 1.65×10^{-6} e Å^{-3} and the isosurface value for the summation of four VB states or CB states is about 4.50×10^{-6} e Å^{-3}.