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Supplementary Information: Near-band-edge exciton polarization change in ZnO nanowires

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Convergence test

An important issue in the calculation of excitonic properties in nanostructures is the treatment of correlations. Our configuration interaction (CI) treatment exhibits a poor scaling, which limits the number of states that we are able to include in the expansion. A careful convergence test is therefore necessary, especially in the case of a NW, where the confinement in the NW direction is the sole result of the electron-hole interaction. The approach followed in this work is to use a large supercell extended in the NW direction, in order to fully include the physical extent of the exciton state, and limit the calculation to the Γ point of the Brillouin zone. An alternative and equivalent approach is to use a minimum supercell size in the NW direction and introduce k-point sampling.

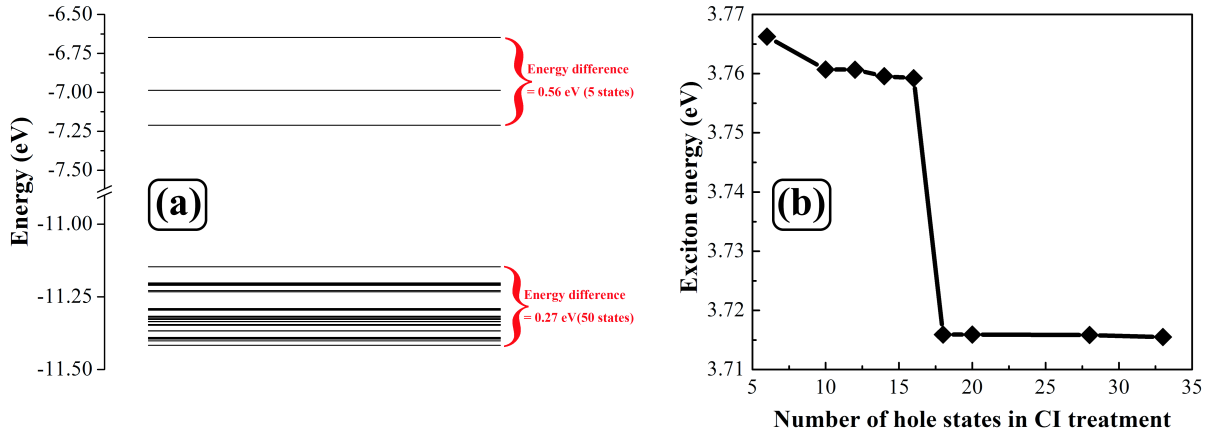

Fig. 1 (a) Single-particle electron and hole energy levels diagram for our smallest ZnO nanowire (with diameter D = 2 nm). Here, we have plotted the first five electron energy levels and the first fifty hole energy levels. (b) Exciton energy as a function of the number of the hole states in the configuration interaction (CI) treatment for our smallest ZnO nanowire (with diameter D = 2 nm). Here, we include the first five electron states in the CI.

For the convergence test, we choose our smallest ZnO nanowire with a diameter D = 2 nm, and plot the corresponding single-particle electron and hole energy levels (see Fig. 1(a)). We find that the single-particle electron states spread in a much larger energy window than its hole states counterparts, e.g., the first five

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electron states distribute in an energy window of 0.56 eV, while the first fifty hole states only spread in a energy window of 0.27 eV. Therefore, we include in our CI treatment the first five electron states and systematically increase the number of hole states. The exciton energy as a function of the number of hole states is presented in Fig. 1(b). As we can see from Fig. 1(b), the exciton energy is insensitive to a further increase of the number of hole states when the number of hole states is larger than eighteen. Thus, we include in our CI treatment five states from the conduction band and eighteen states from the valence band.