

## Supplementary Materials

The effect of size on the electronic and anti-corrosion properties is considered by increasing the size of the ZHEX-ZnO quantum dots to 4ZHEX-ZnO and 5ZHEX-ZnO as seen in Fig. S1 (a, d). The corresponding HOMO and LUMO distributions are shown in (b,c) and (e, f) respectively. It is observed that the HOMO and LUMO are distributed on the edges of the nanodots with localized distribution on a few atoms. This means that the HOMO and LUMO originate from interactive edge states that decrease the energy gap than even the periodic structure.

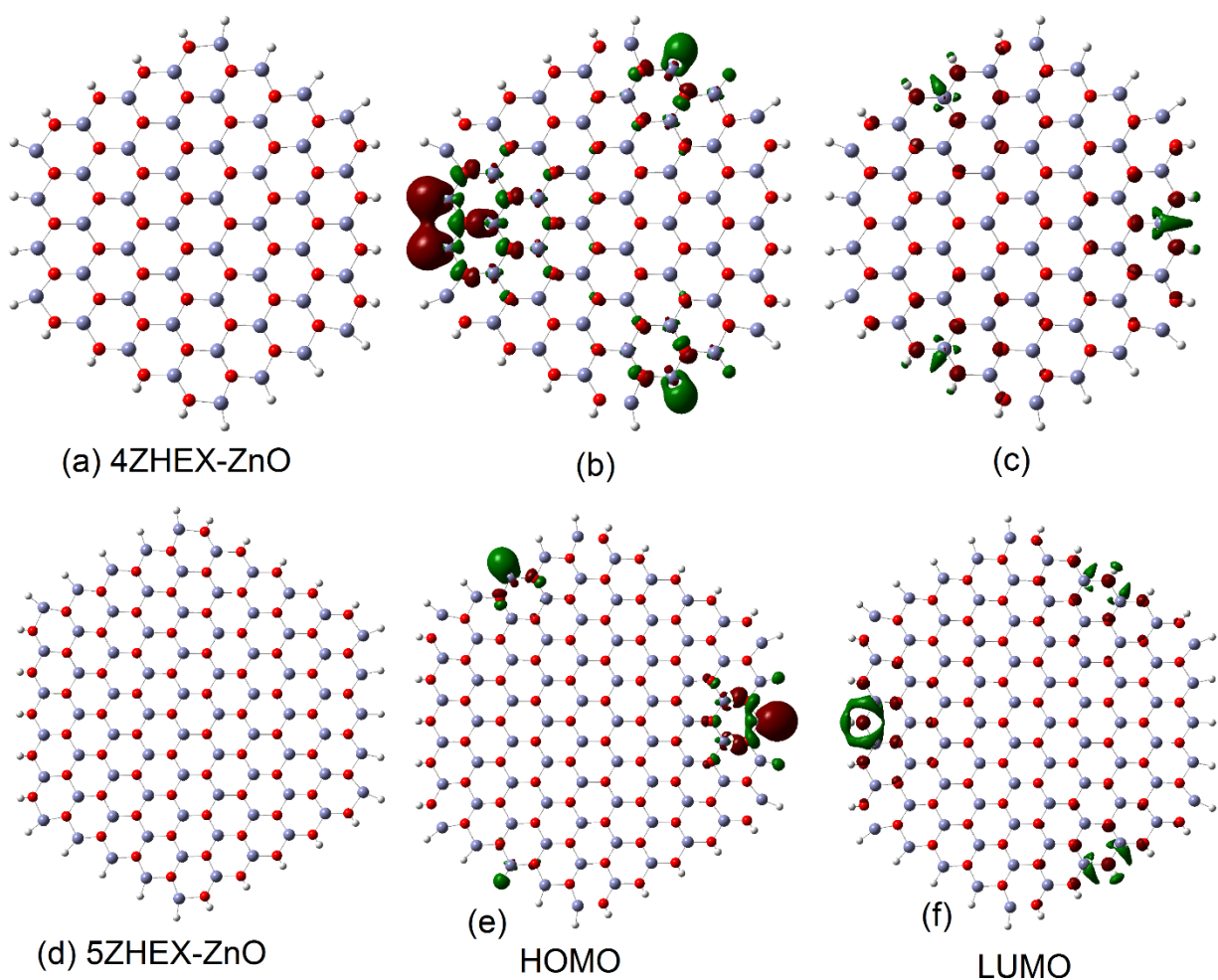


Figure S1. The optimized structures of ZnO nanodots with four (4ZHEX-ZnO) and five (5ZHEX-ZnO) edge hexagons, see (a) and (d), respectively. The related HOMO and LUMO distributions of 4ZHEX-ZnO are shown in (b,c) and those for 5ZHEX-ZnO are shown in (e,f).

The periodic calculations of the 2D ZnO crystal (Fig. S2 a) are provided here to extend our investigations to include the infinite 2D structure and compare with the experimental results. The calculated density of states (DOS) shown in Fig. S2 (b) indicates that the contribution of O-atoms to the total density of states is higher than that of Zn atoms, especially the low energy peaks. This result is confirmed by the distributions of the highest occupied/lowest unoccupied crystal band (HOCB/LUCB) where the extended yellow cubes

are distributed mostly on O-atoms. It is noted that the distribution on the Zn atoms is slightly higher in LUCB than in HOCB which consists also with the DOS distribution where the small peak representing the LUCB has almost the same contribution from both Zn and O atoms. It is also noted that the energy gap equals 3.43 which is lower than the experimental one of 4.48 eV obtained by Lee et al.[1]. Nevertheless, our results are in good agreement with previous theoretical calculations using the HSE functional [1,2].

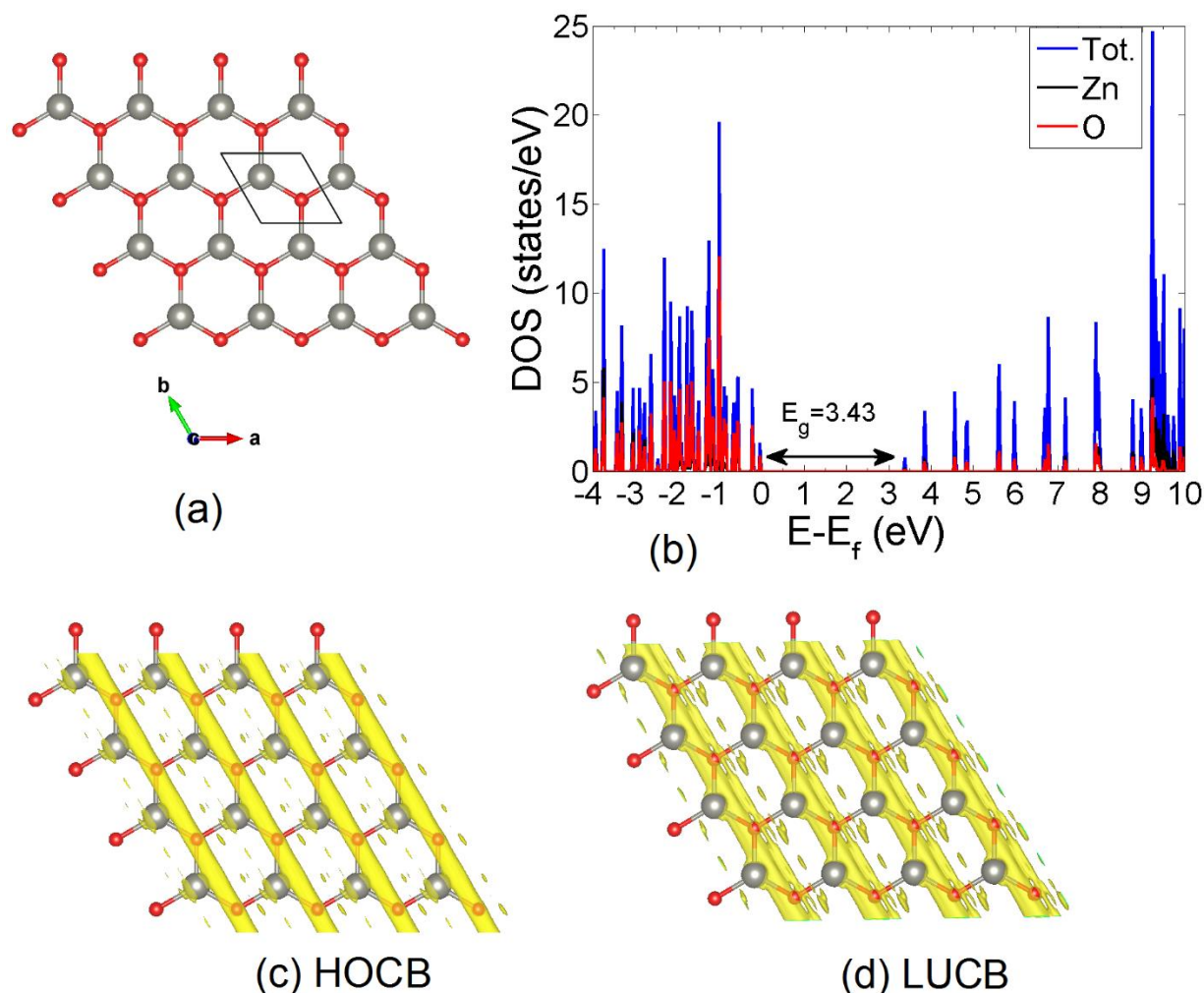


Figure S2. (a) top view of the two-dimensional ZnO lattice with the unit cell indicated by the box. (b) the total and partial density of states. (c,d) The highest occupied/lowest unoccupied crystal band (HOCB/LUCB). The colors of the Zn and O atoms are displayed as gray and red, respectively.

## References

1. Lee, J.; Sorescu, D.C.; Deng, X. Tunable lattice constant and band gap of single-and few-layer ZnO. *The journal of physical chemistry letters* **2016**, 7, 1335–1340.
2. Zhao, Y.; Liu, N.; Zhou, S.; Zhao, J. Two-dimensional ZnO for the selective photoreduction of CO. *Journal of Materials Chemistry A* **2019**, 7, 16294–16303.