Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information

Exponential size-dependent tunability of strain on the transport behavior in ZnO tunnel junctions: An ab initio study

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I. Supplementary figures

Figure. S1 The deformation charge density on (110) plane of 'h_t' PTJs with different ZnO barrier thickness (*m* ranging from 2 to 5).

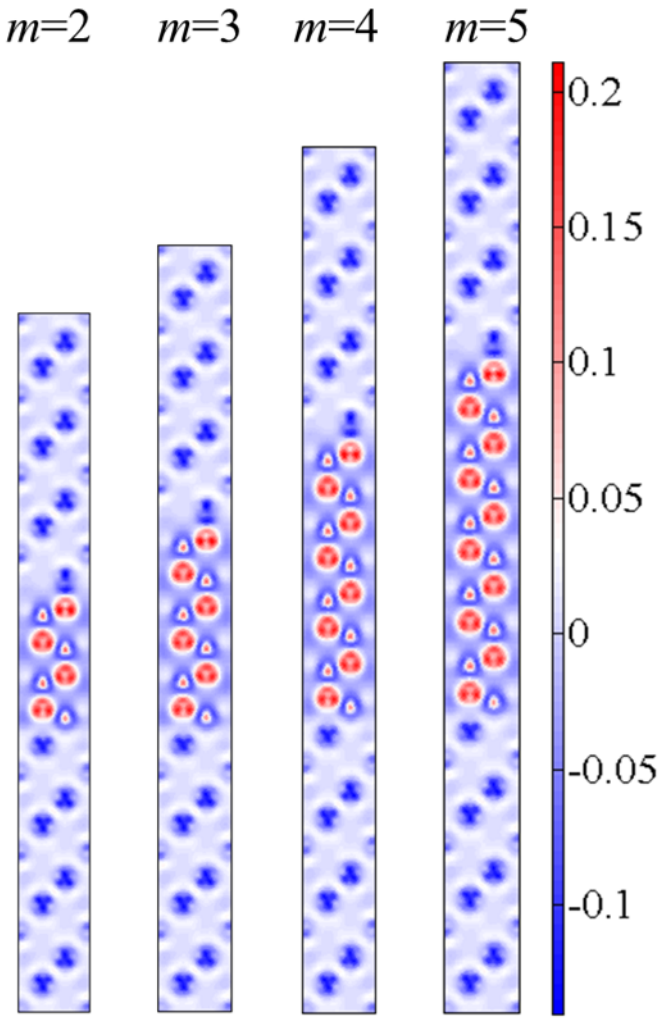
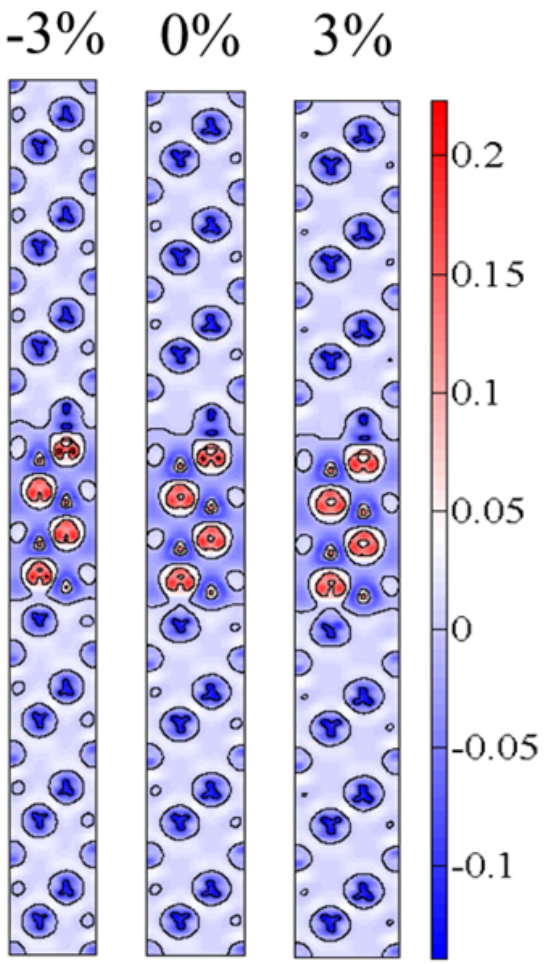


Figure. S2 The deformation charge density on (110) plane of 'h_t' PTJs with *m*=2 under different strain (i.e., -3%, 0% and 3%). The in-plane compressive (tensile) strain leads to the stretch (shortening) of ZnO PTJs along *z*-axis.



II. A Comparison between the GGA+U and Heyd-Scuseria-Ernzerh of screened hybrid density functional (HSE) method

Calculations of ZnO using Heyd-Scuseria-Ernzerh of screened hybrid density functional (HSE) method have been performed by researchers[1]. Here, we make a comparison between the GGA+U and HSE results. Both of the two methods give accurate in-plane lattice parameters of wurtize ZnO (3.28Å and 3.25Å), which is closed to the experimental result (3.24Å).The band gap of ZnO in our GGA+U calculations is 2.13eV, which is also quite closed to the result obtained with HSE method (2.50eV). It's thought that the improvement of accuracy in calculation the band gap with GGA+U method mainly results its good description of Zn 3d orbits. The Zn 3d electrons in our GGA+U calculation are mainly localized around 5.7eV below the valence band edge, which is quite closed to the HSE results (6.0eV). In addition, the energy range of Zn 3d orbits (3.0eV) in our calculation is a little larger than that of the HSE calculation (2.2eV). Based on these comparisons, we think that the results by GGA+U methods in our work are reliable.

Reference

1. J. Wróbel, K. J. Kurzydłowski, K. Hummer, G. Kresse and J. Piechota, *Phys. Rev. B*, 2009, **80**, 155124.