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

Supplemental Materials for

Enhancing thermoelectric performance of gamma-graphyne nanoribbons by introducing edge disorder

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1. Comparing between tight-binding results and density functional tight-binding method

To validate the reasonability of our results, we recalculate the thermoelectric properties of edge-disordered gamma-graphyne nanoribbons (γ-GYNR) by utilizing the density functional tight-binding method as implemented in the DFTB+ software[1]. It can be seen from figure. S1 that the thermoelectric figure of merit ZT of γ-GYNRs obtained from the TB parameters and DFTB+ software shares almost same value and similar trends with different edge disorder magnitudes. That is to say, the TB parameters employed in our calculation could be qualitatively extended to study the thermoelectric performance of edge-disordered γ-GYNRs.

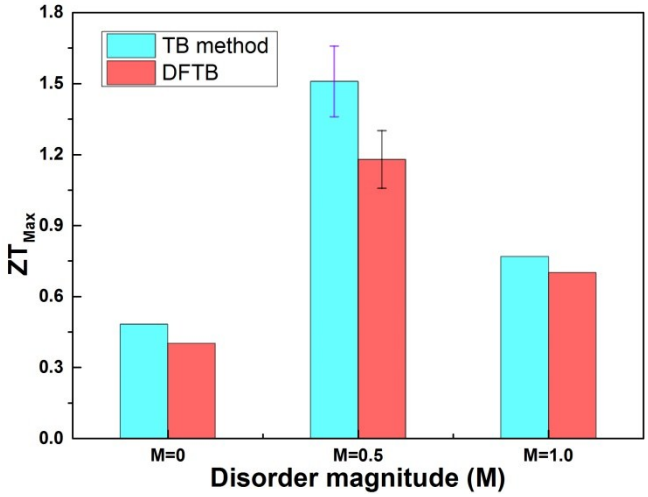

Figure S1. The room temperature maximum value of thermoelectric figure of merit ZT for γ-GYNR (width and length of central region is 1.41 and 13.92 nm) with different edge disorder magnitude.

Reference

1. B. Aradi, B. Hourahine and T. Frauenheim, *The Journal of Physical Chemistry A*, 2007, **111**, 5678-5684.