Theoretical investigation of width effect in electronic and transport properties of carbon nanoribbons with 5-8-5 carbon rings: a first principle study

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Supporting Information (SI)



Fig. S1. Comparative of I-V curve for all molecular devices: (a) (9,w)zzP1, (b) (9,w)zzO, (c) (9,w)zzP2, (d) (5,w)acP, and (e) (5,w)acPO. We clearly see that the I values of zz nanoribbons are higher than ac cases.



Fig. S2. Comparative of (dI/dV)-V curve for all molecular devices: (a) (9,w)zzP1, (b) (9,w)zzO, (c) (9,w)zzP2, (d) (5,w)acP, and (e) (5,w)acPO. We clearly see that the conductance of zz nanoribbons are higher than ac cases.