Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information for:

Negative differential resistance behavior of Si/B-substituted into a C_6 chain sandwiched between capped carbon nanotube junctions

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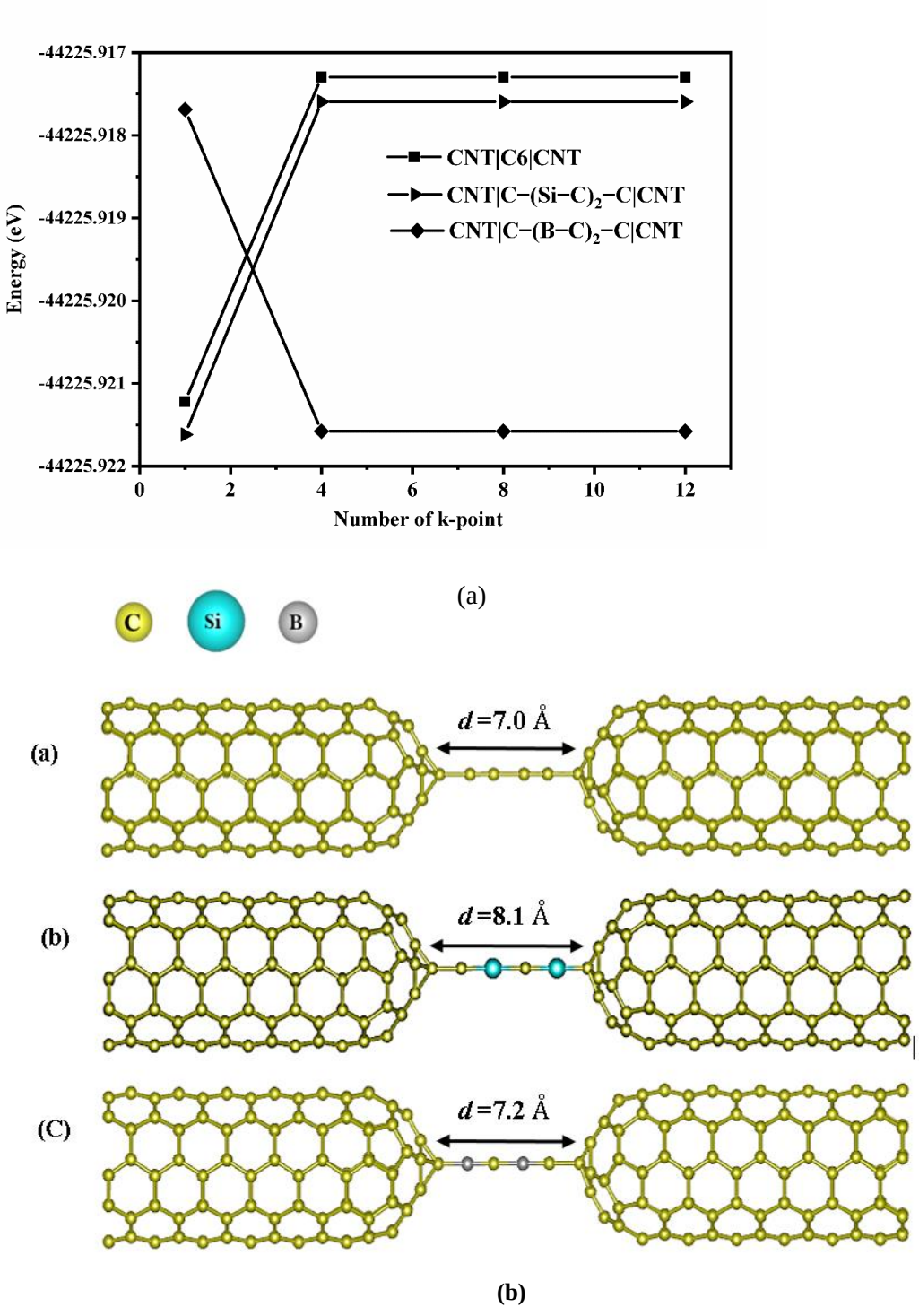


Fig. S1: (a) Energy (eV) vs. number of k-points for CNT|C6|CNT, CNT|C−(Si−C)$_2$−C|CNT and CNT|C−(B−C)$_2$−C|CNT molecular devices, (b) (b) Initial geometries of (a) C_6, (b) C−(Si−C)$_2$−C and (c) C−(B−C)$_2$−C junctions with CNTs electrodes.

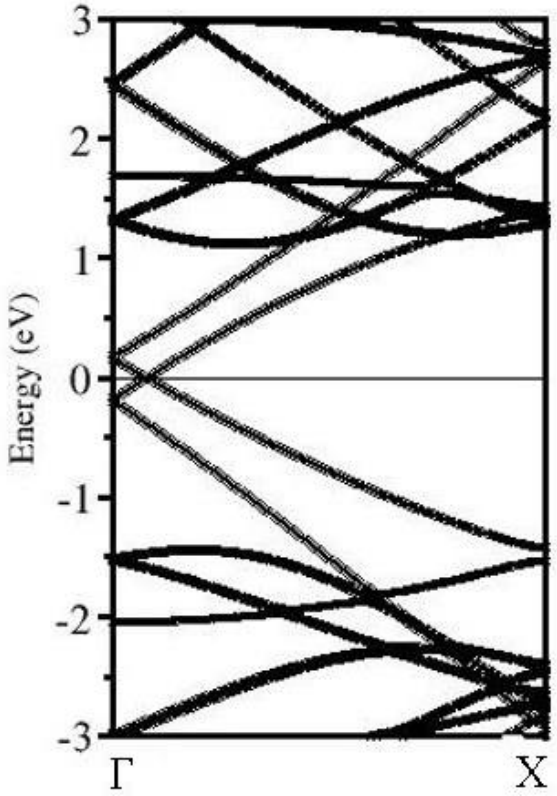


Fig. S2: (a) Band structure of CNT electrodes (including five nanotube lead layers). The Fermi level is set to zero. The solid line represents the Fermi level.

CNT|C6|CNT

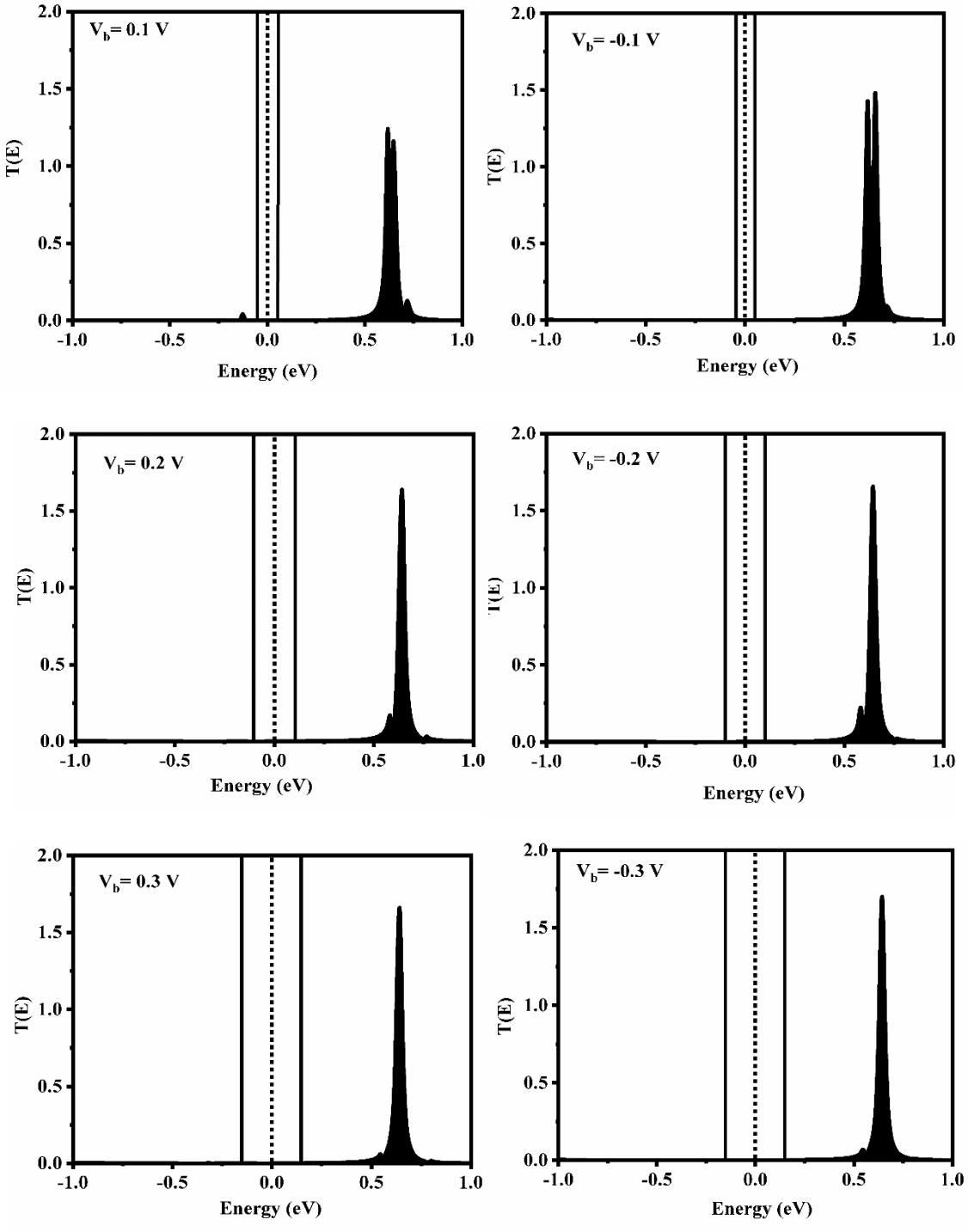


Fig. S3: Bias-dependent transmission spectra of (a) CNT|C_6|CNT, (b) CNT|C−(Si−C)$_2$−C|CNT, and (c) CNT|C−(B−C)$_2$−C|CNT molecular devices. The Fermi level is set to zero. The dotted lines represent the Fermi level. The energy regions between the two solid lines show the bias window.

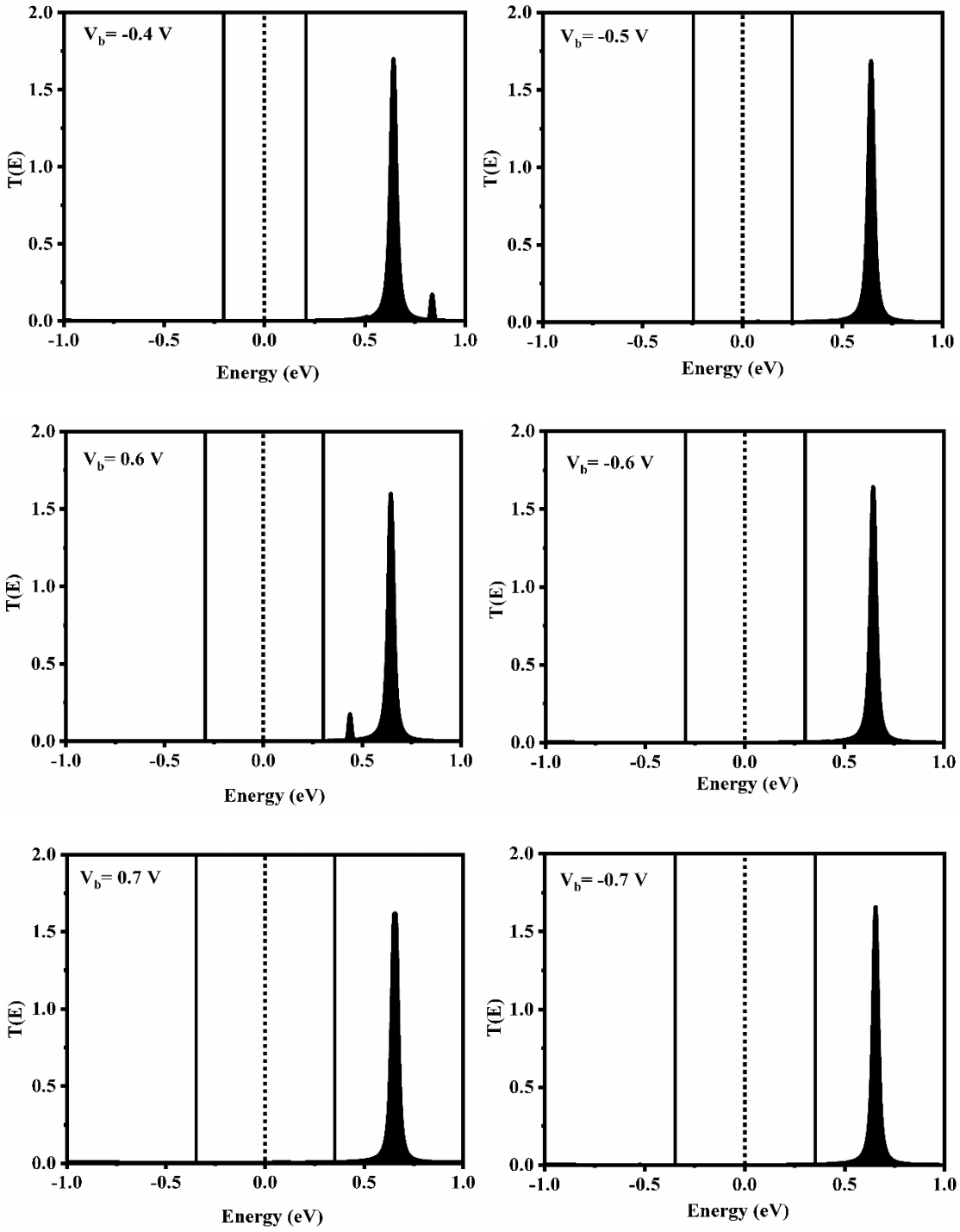
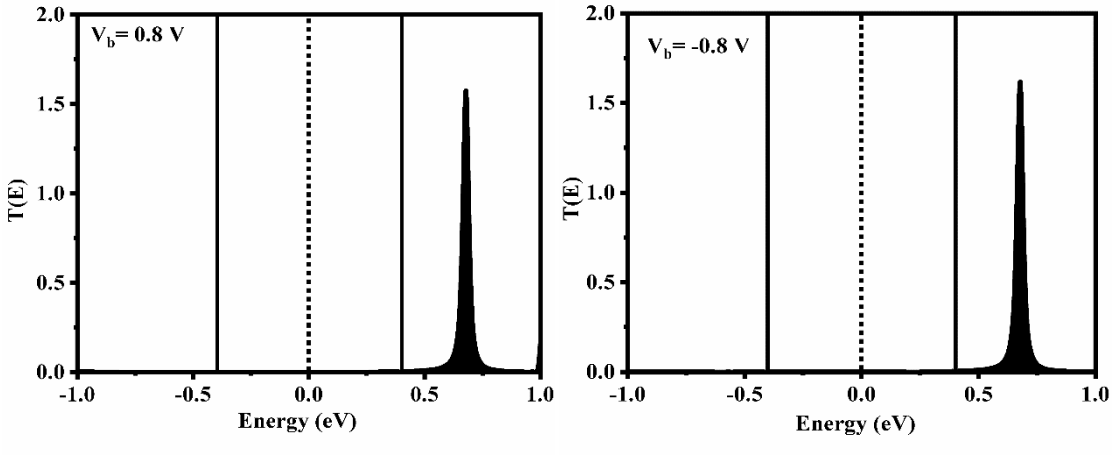


Fig. S3: continued



(a) CNT|C−(Si−C)$_2$−C|CNT

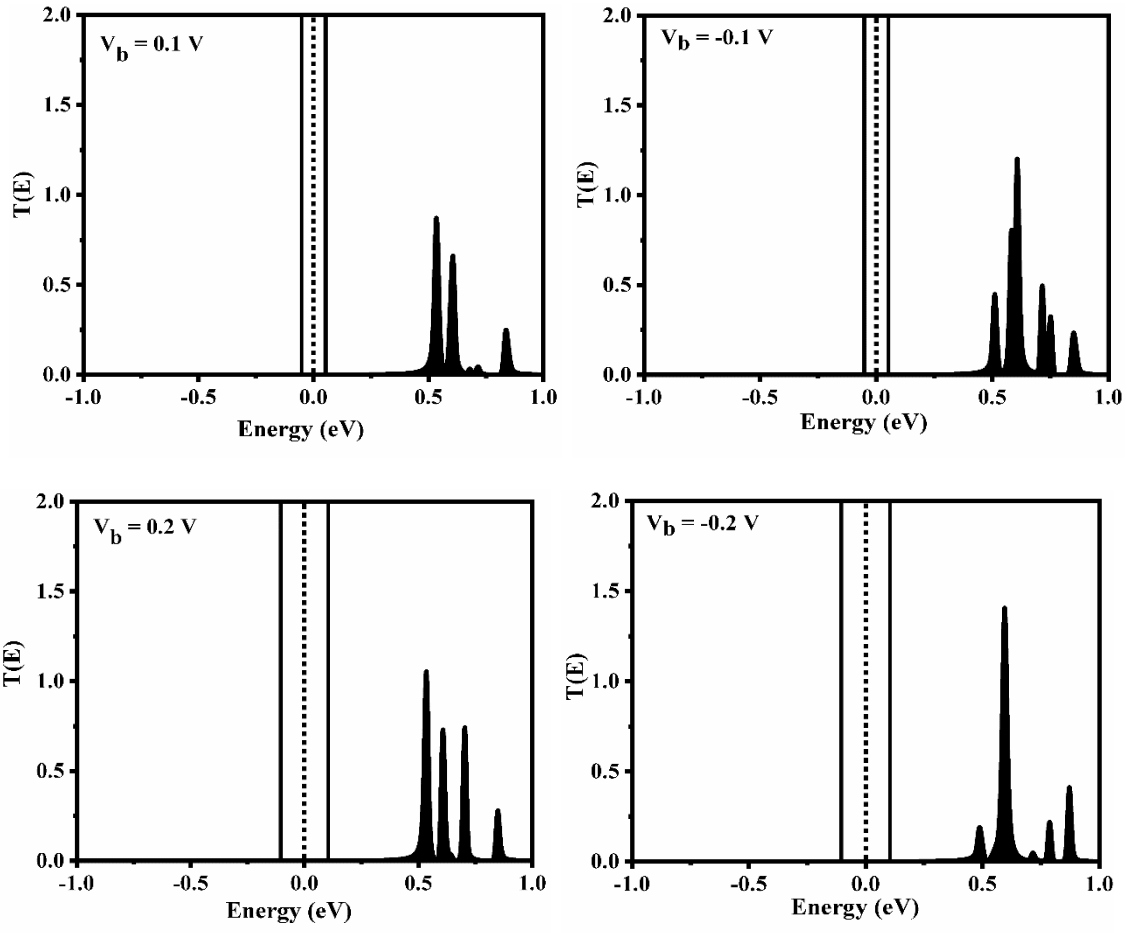


Fig S3: continued

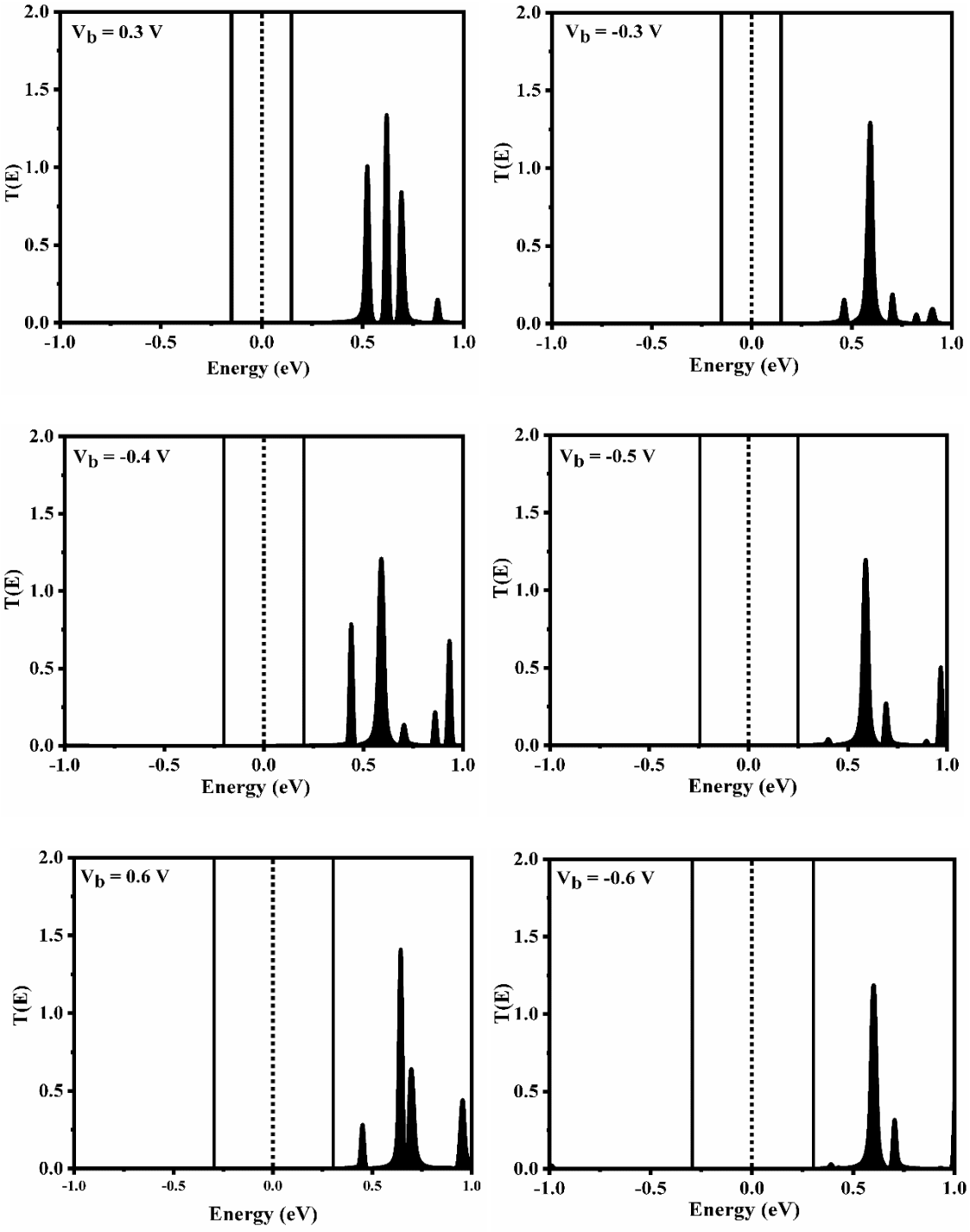
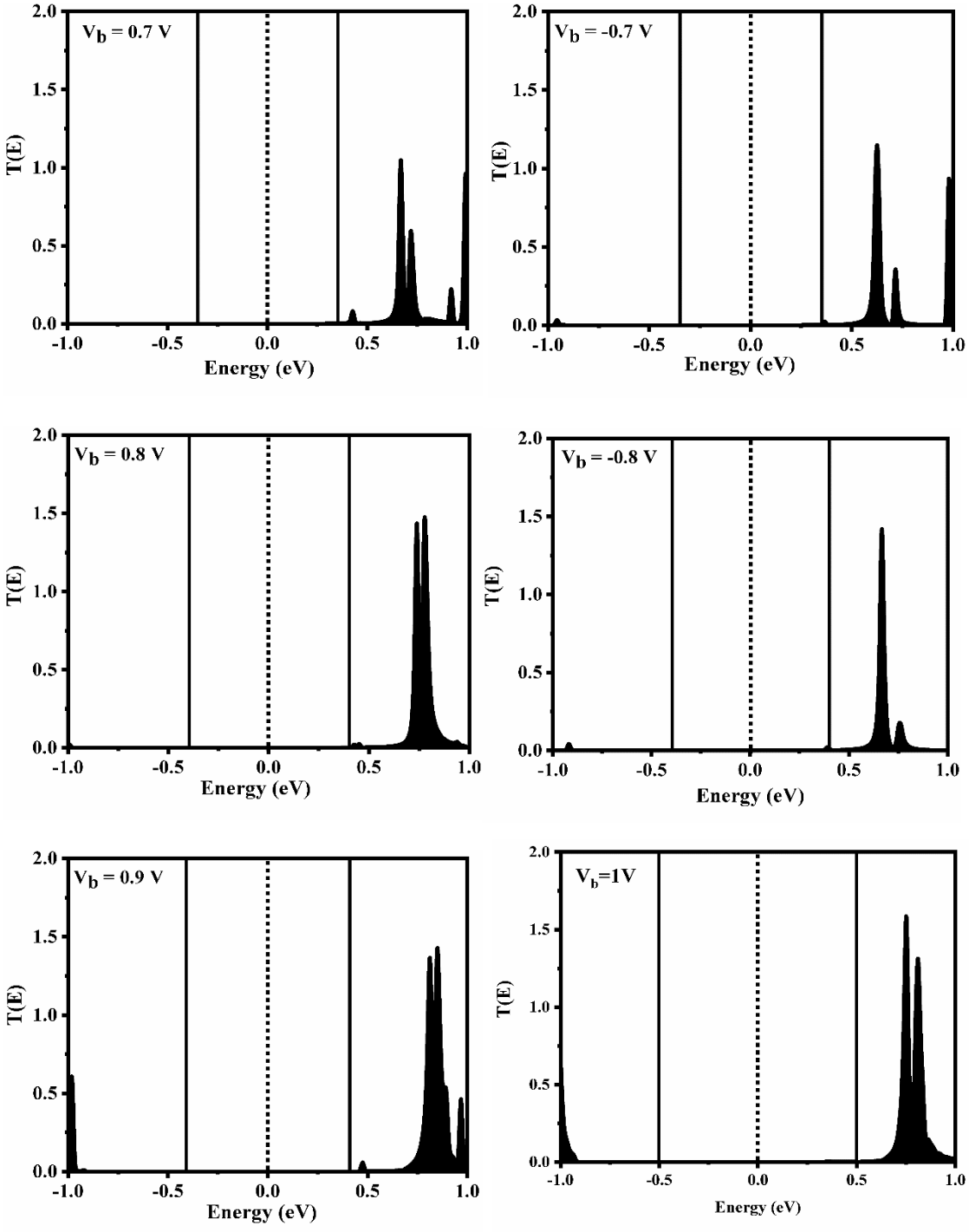


Fig S3: continued



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(b) CNT|C−(B−C)$_2$−C|CNT

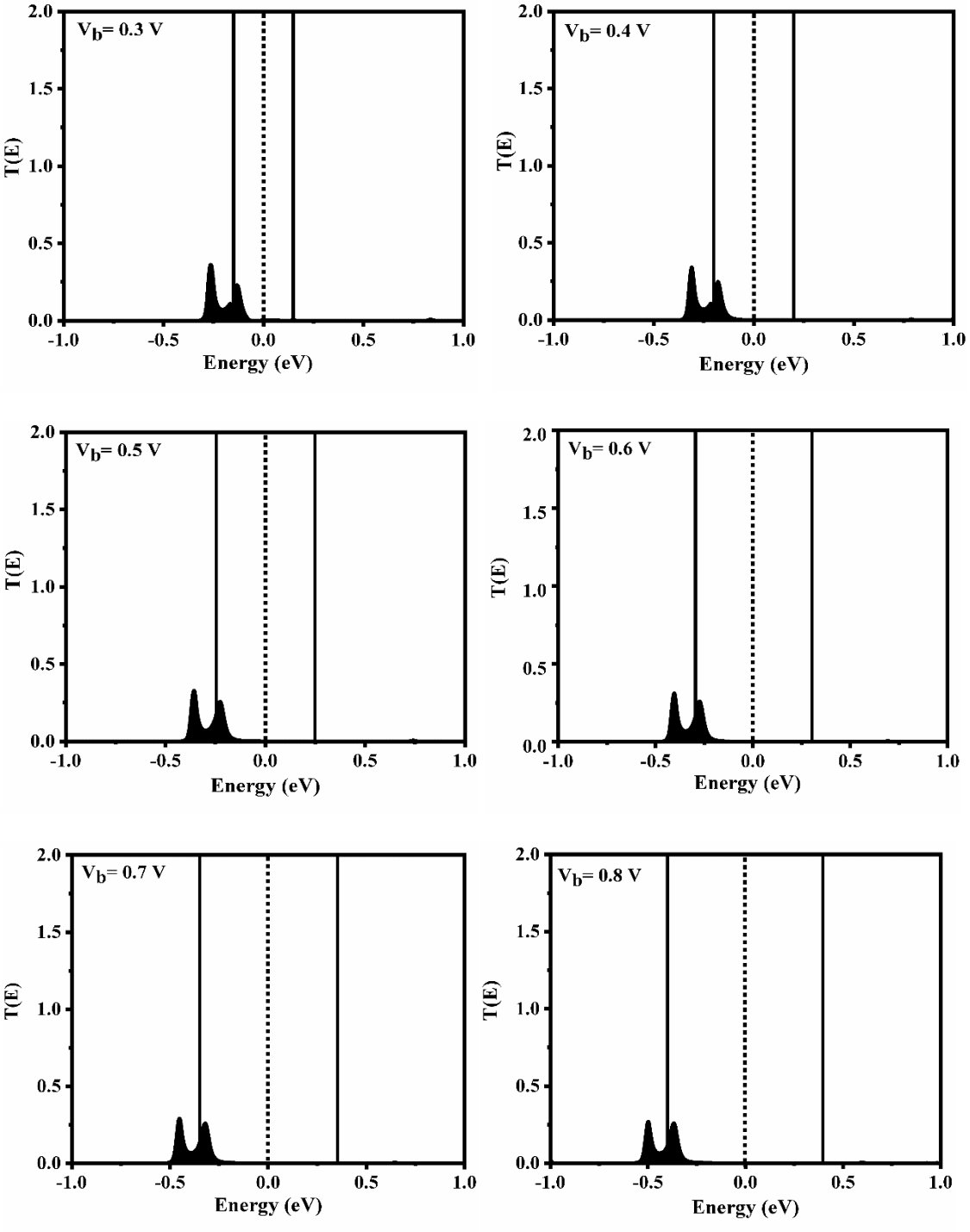

Fig S3: continued

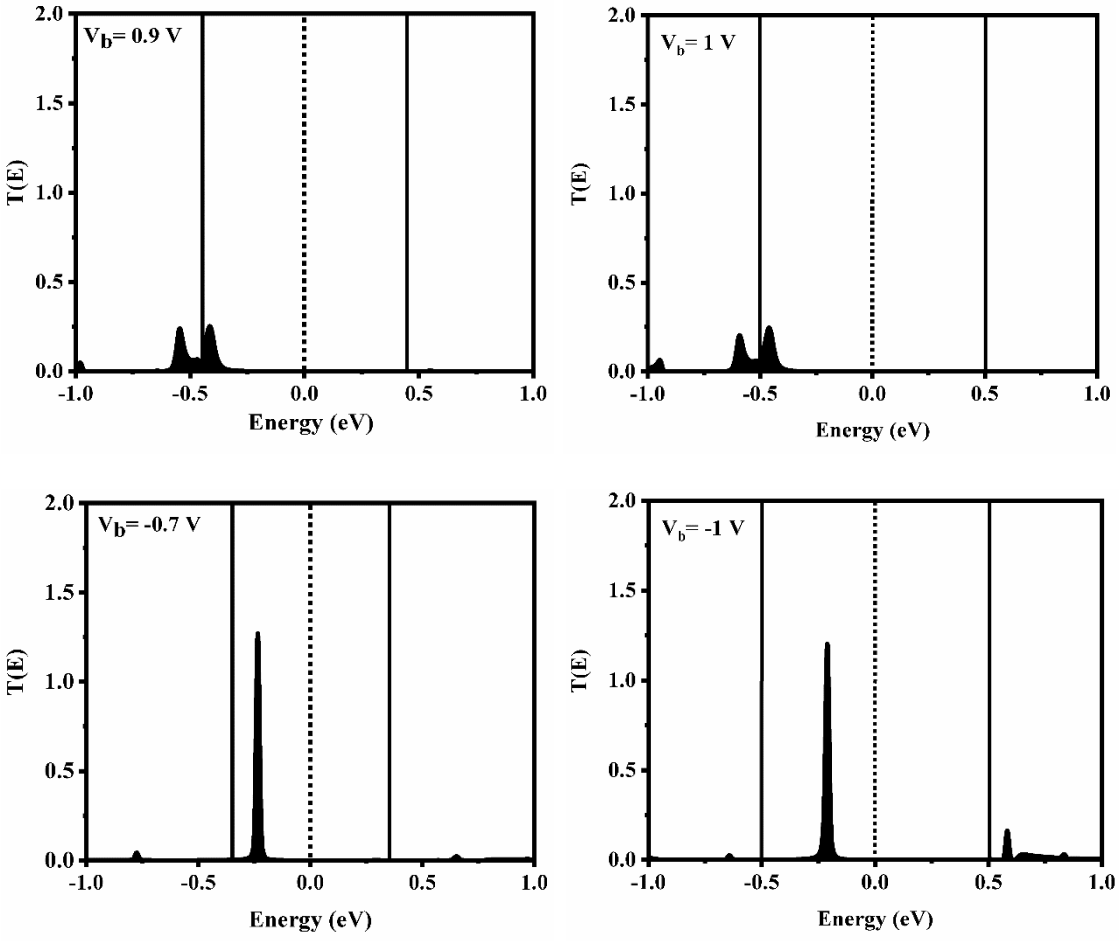

Fig S3: continued