

Supporting Information: Effect of packing motifs on the energy ranking and electronic properties of putative crystal structures of tricyano-1,4-dithiino[c]-isothiazole

Farren Curtis^a, Xiaopeng Wang^b, and Noa Marom^{a,b*}.

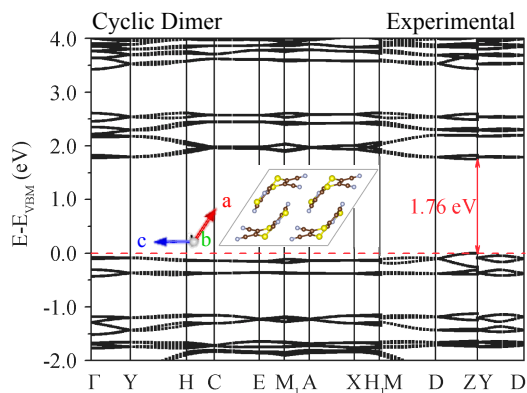
^a*Department of Physics, Carnegie Mellon University, Pittsburgh, PA 15213, USA.* ^b*Department of Materials Science and Engineering, Carnegie Mellon University, Pittsburgh, PA 15213, USA.*

Table S1: Closest C \cdots N, S \cdots N, C \cdots C, and S \cdots S contacts for representative putative crystal structures of TCS3.

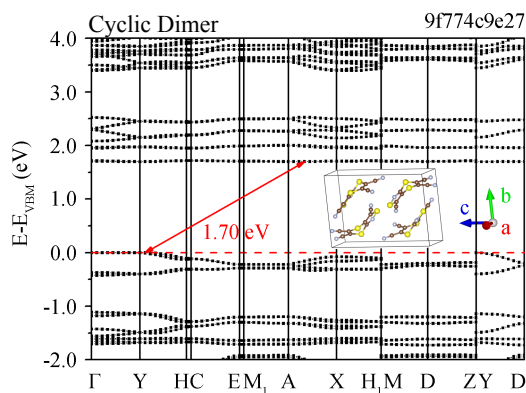
Label	C \cdots N (Å)	S \cdots N (Å)	C \cdots C (Å)	S \cdots S (Å)
<i>P2</i> ₁ / <i>n</i> Cyclic Dimer	3.02	3.27	3.36	3.74
<i>P2</i> ₁ / <i>c</i> Cyclic Dimer	3.13	3.30	3.42	3.81
<i>Pna2</i> ₁ Bilayer	3.04	3.03	3.57	3.66
<i>P2</i> ₁ 2 ₁ 2 ₁ Bilayer	3.02	3.00	3.43	3.59
<i>P2</i> ₁ / <i>c</i> Planar	3.00	2.93	3.45	3.45
<i>P2</i> ₁ Catemer	3.18	3.15	3.70	3.93
<i>Pna2</i> ₁ Catemer	3.14	3.10	3.58	3.82

*Corresponding author: nmarom@andrew.cmu.edu

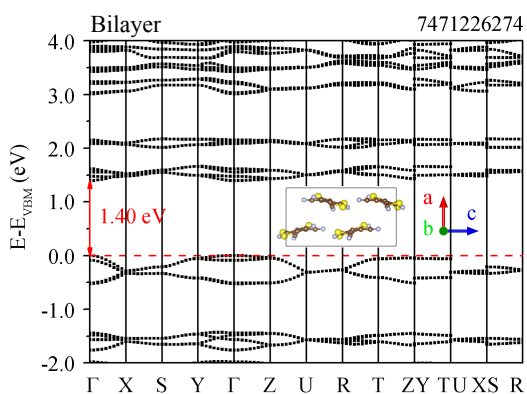
Figure S1: The PBE band structures of the top 36 non-duplicate PBE0+MBD ranked structures (including the experimental structure), with the original labels used from the submission to the sixth blind test. The labeling used for representative structures discussed within the main article have the following equivalent names: $P2_1/n$ cyclic dimer= experimental (panel a), $P2_1/c$ cyclic dimer= 9f774c9e27 (panel b), $Pna2_1$ Bilayer = 7471226274 (panel c), $P2_12_12_1$ Bilayer = dab6897b90 (panel d) $Pna2_1$ Catemer = 42a9600b47 (panel e). $P2_1$ Catemer = d037ff743 (panel f), $P2_1/c$ Planar = 52cdef12ff (panel z).



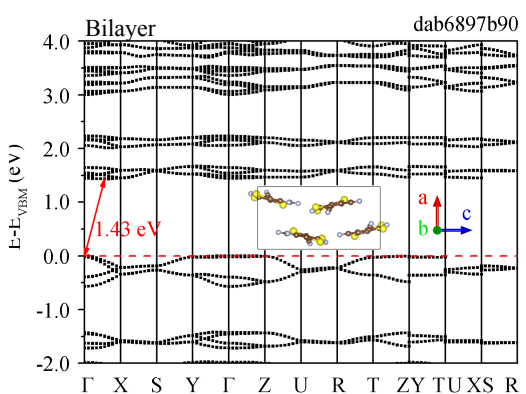
(a)



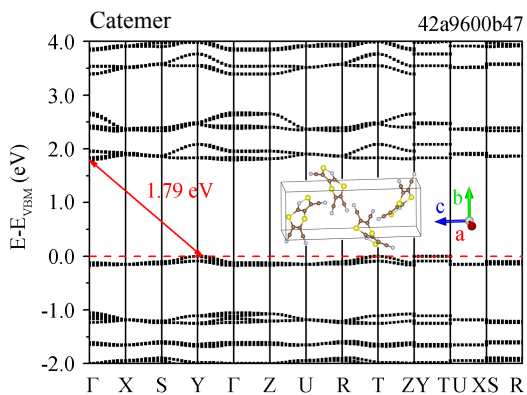
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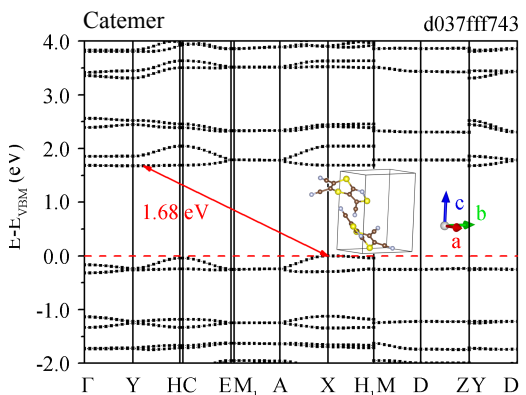
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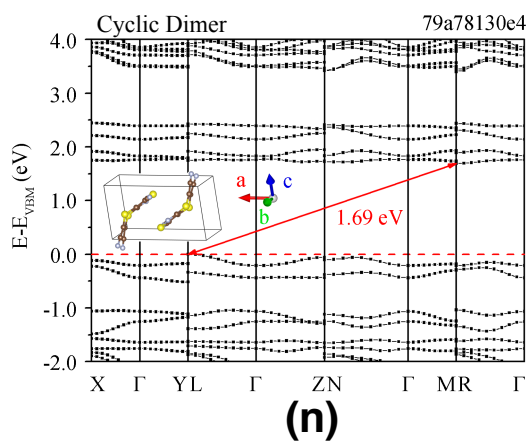
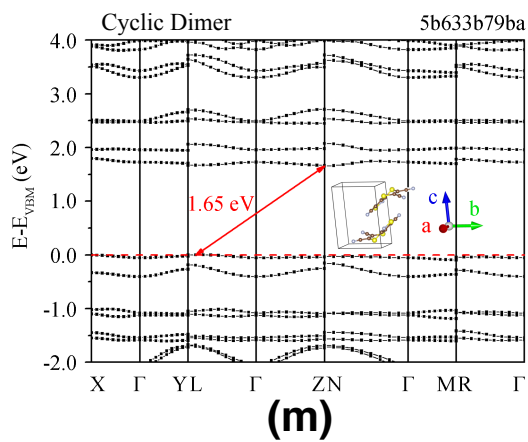
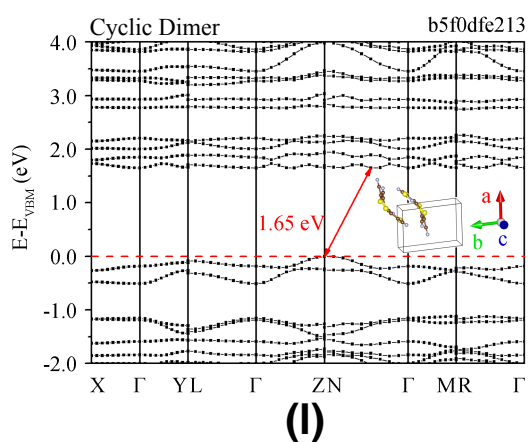
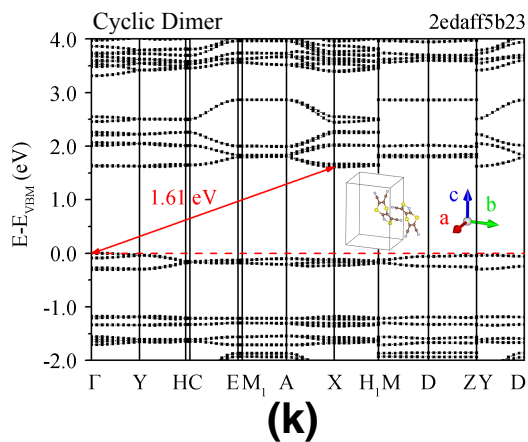
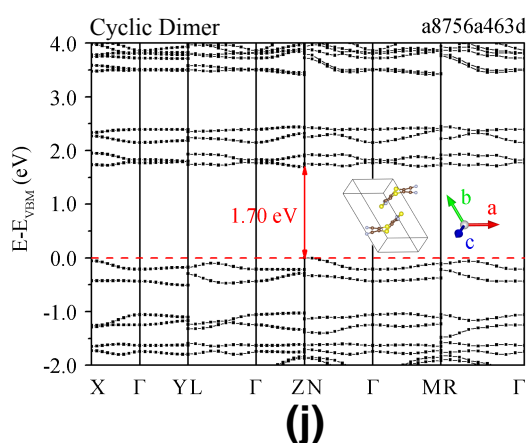
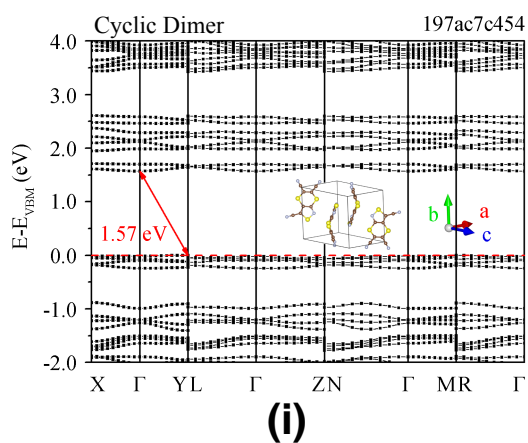
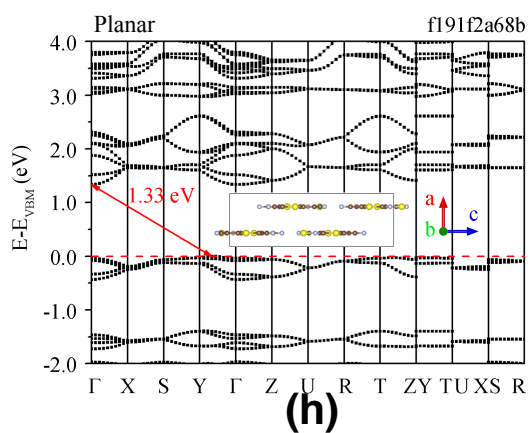
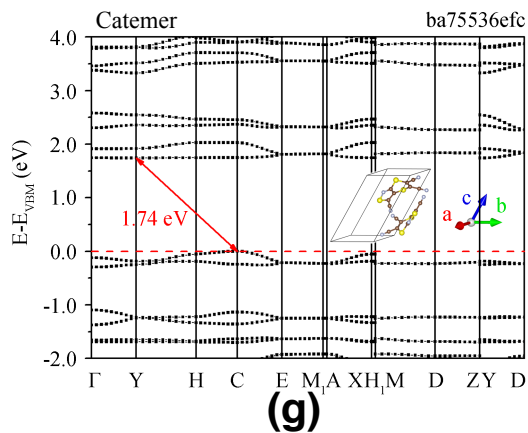
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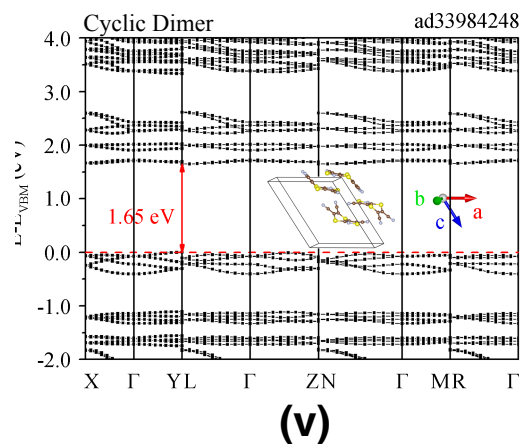
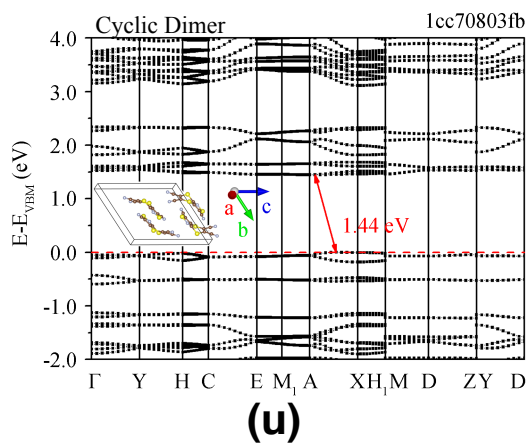
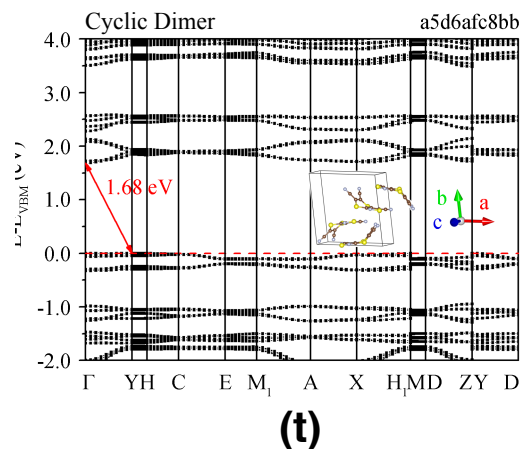
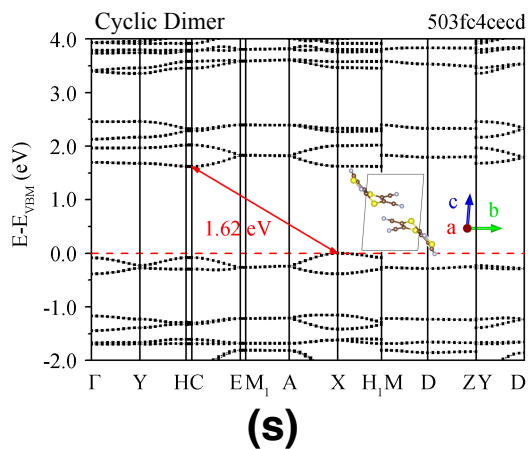
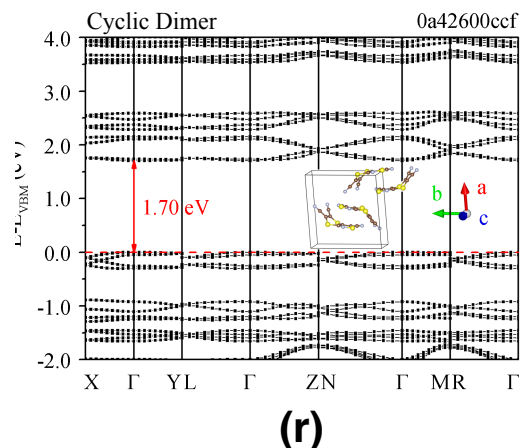
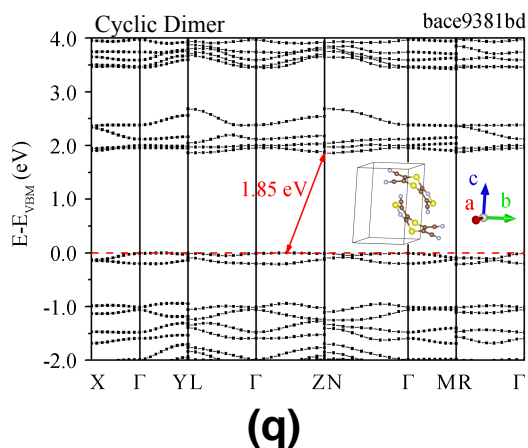
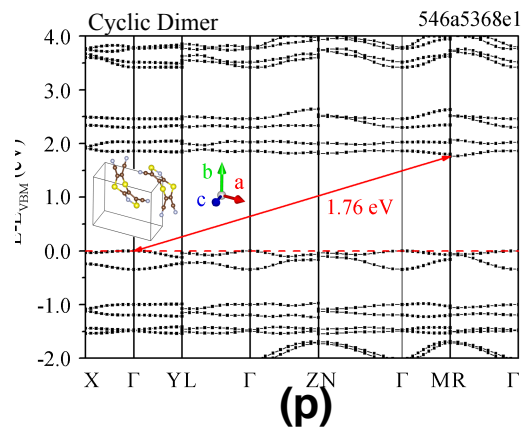
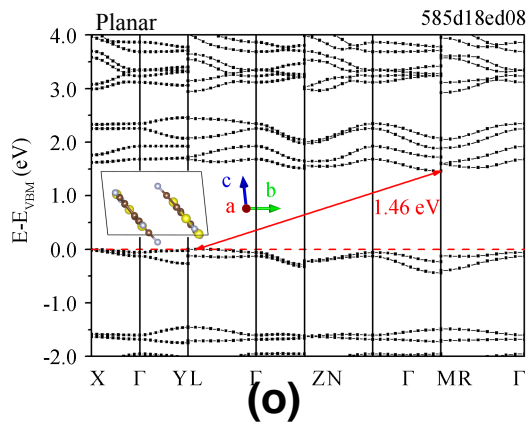


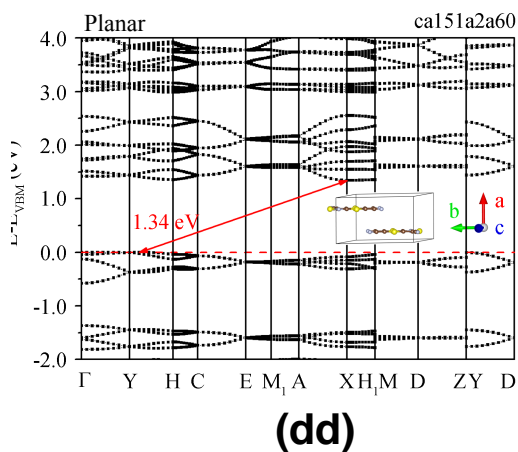
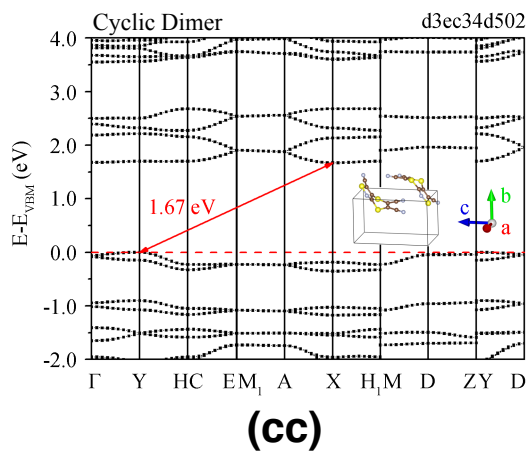
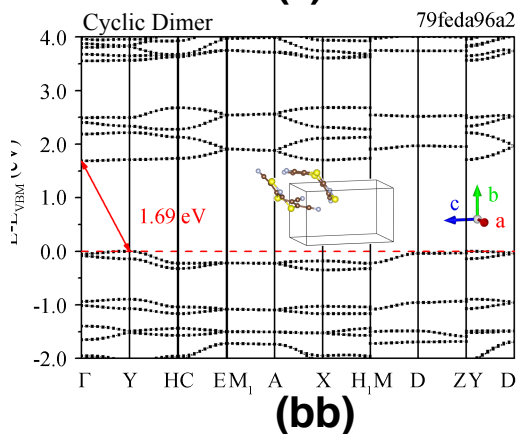
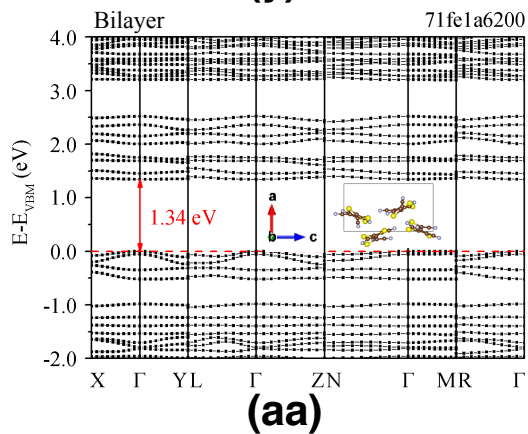
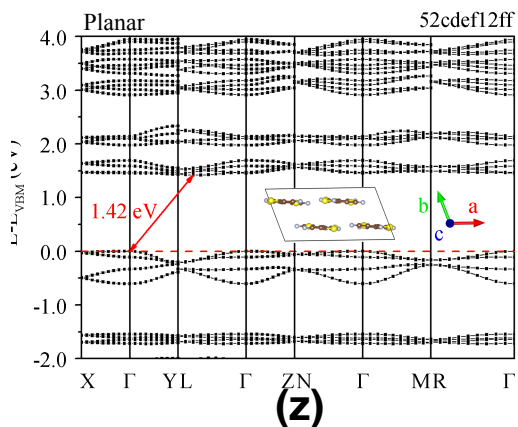
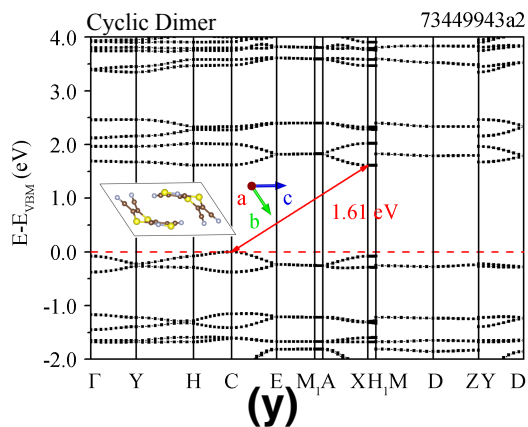
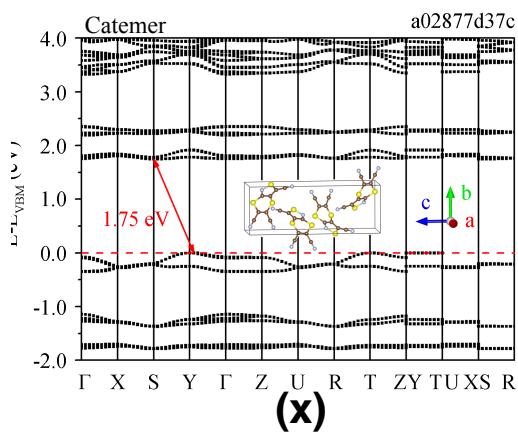
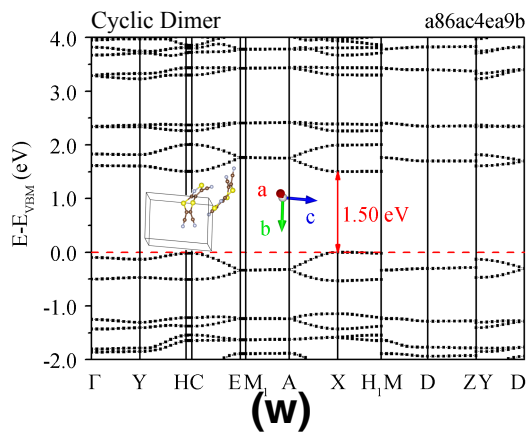
(e)

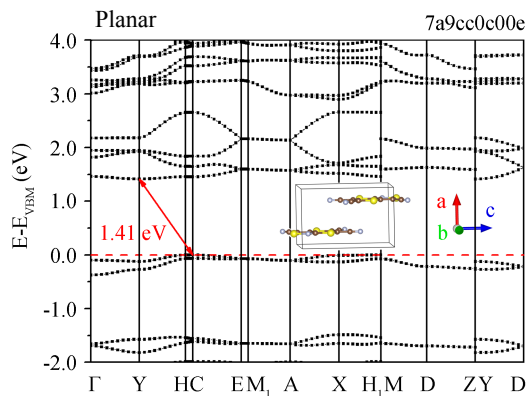


(f)

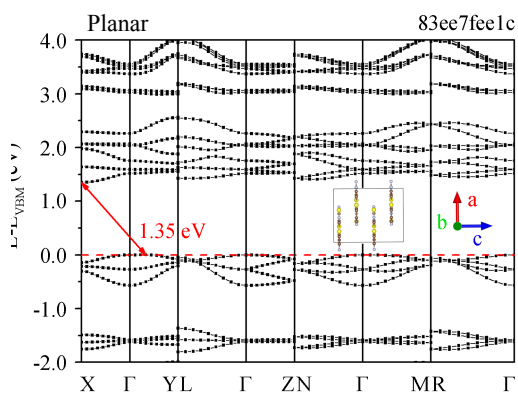




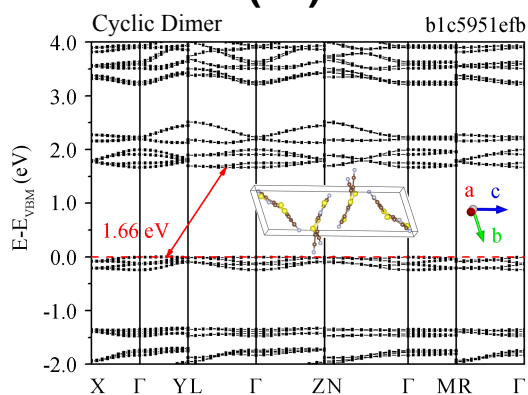




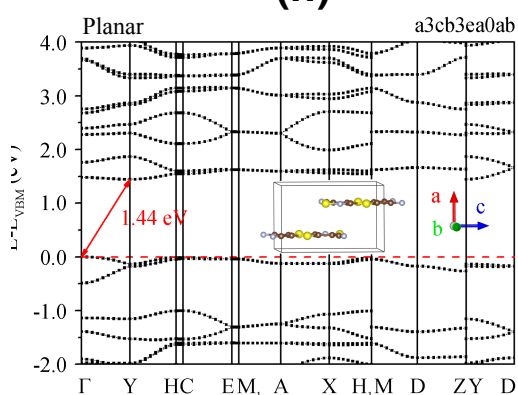
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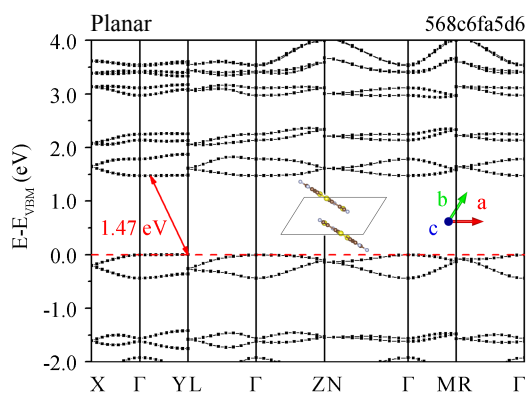
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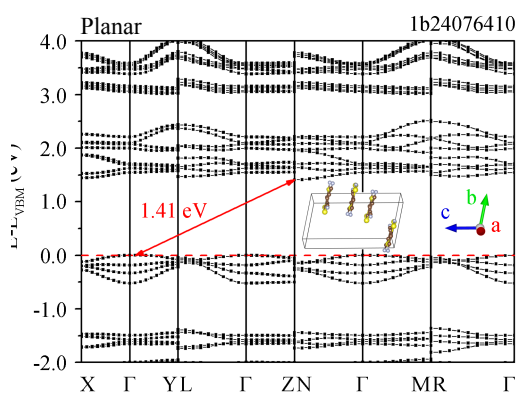
(gg)



(hh)



(ii)



(ji)