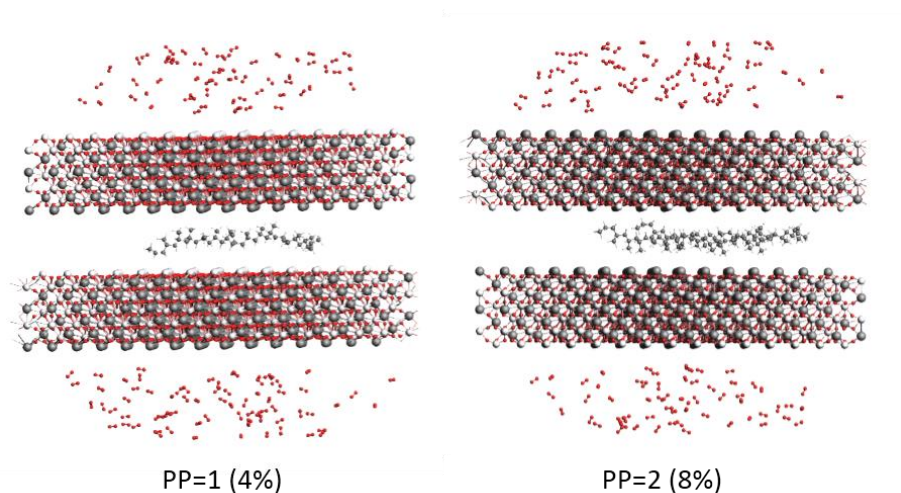


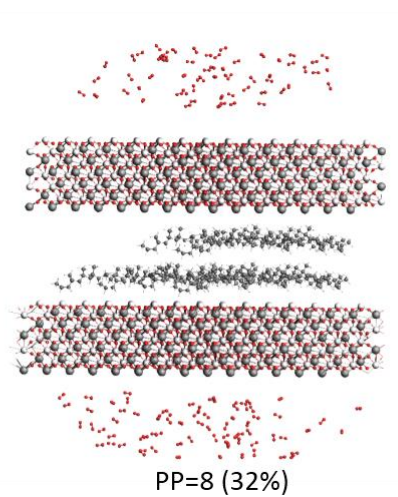
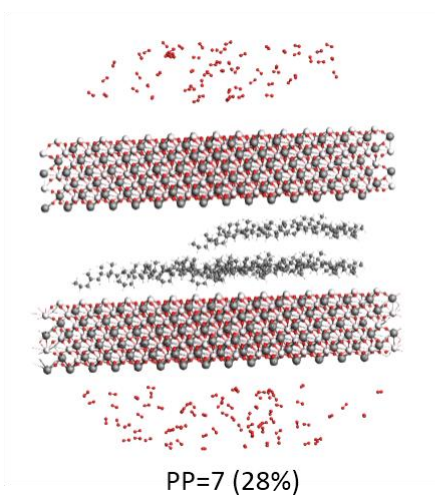
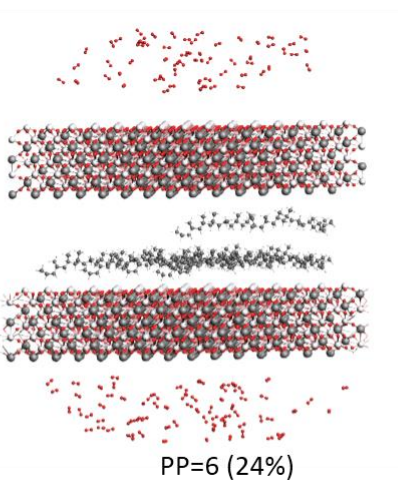
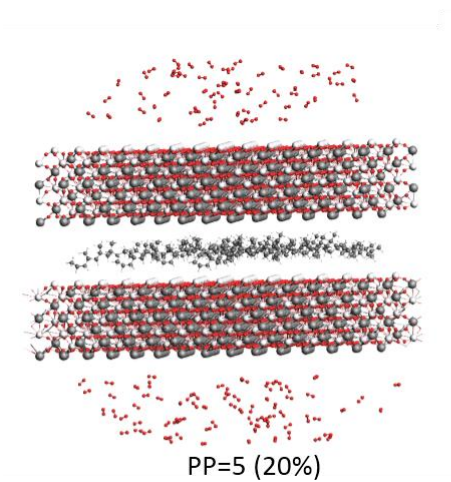
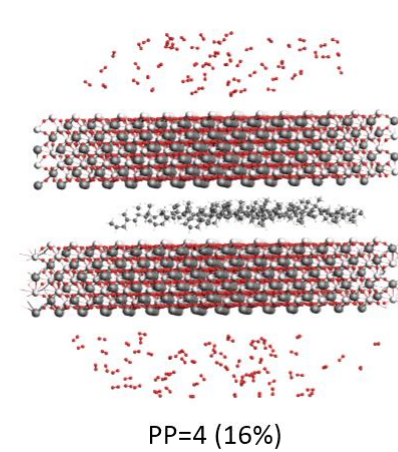
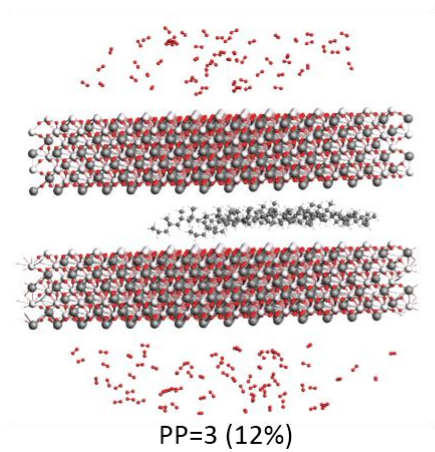
# Supplementary Materials

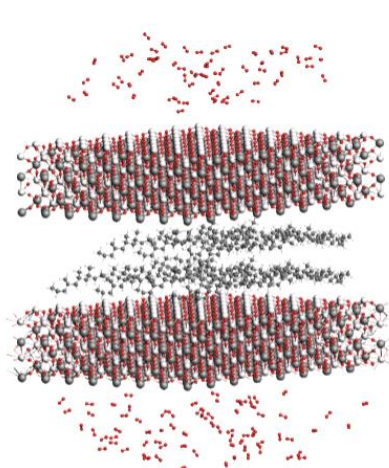
## A Molecular Understanding over the Flame Retardant Mechanism of Zinc Stannate/Polypropylene Composites via ReaxFF Simulations

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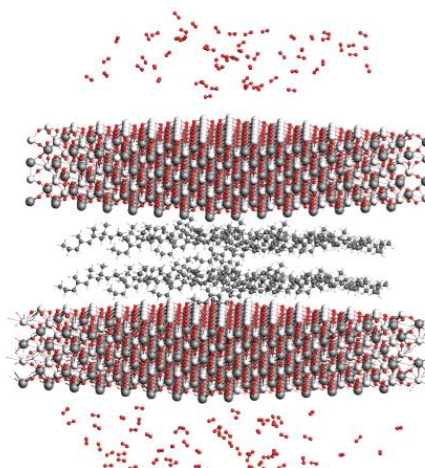
1. Yunnan Tin Industry Group (Holding) Co. Ltd. R & D Center, Kunming, 650200, China
  2. College of Basic Medical Sciences, Ningxia Medical University, Yinchuan 750004, China
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- \* Corresponding authors: C. Geng (Email: gengchang1111@163.com), H. Bai (E-mail: hongcunbai@nxu.edu.cn)



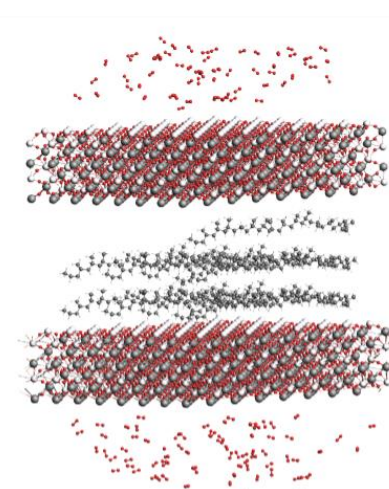




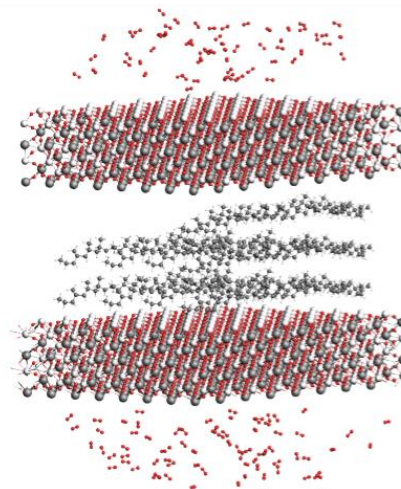
PP=9 (36%)



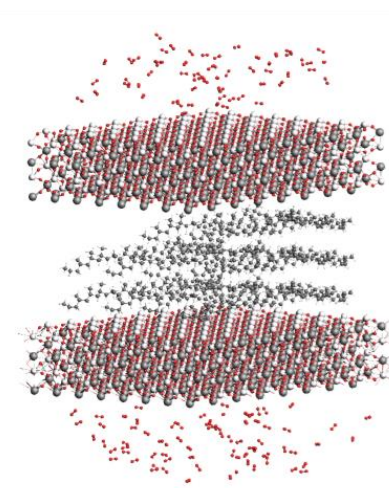
PP=10 (40%)



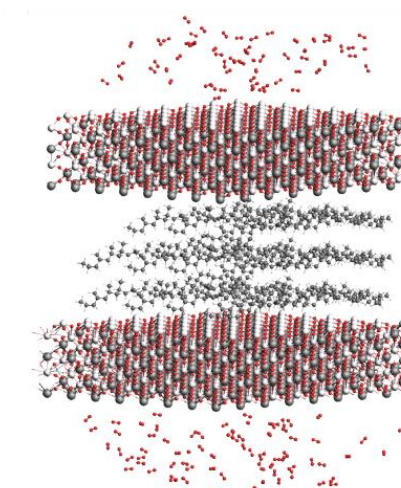
PP=11 (44%)



PP=12 (48%)

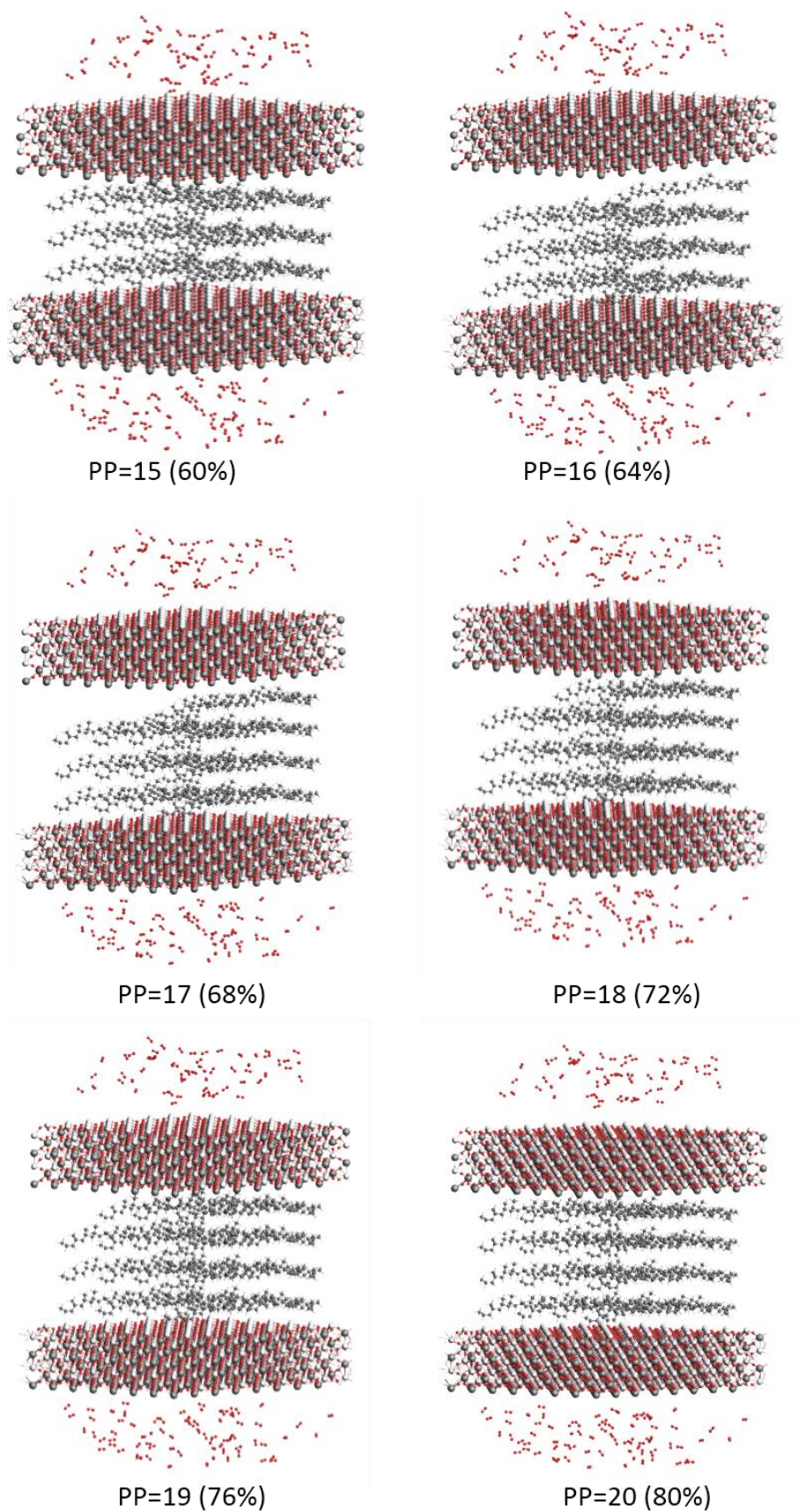


PP=13 (52%)

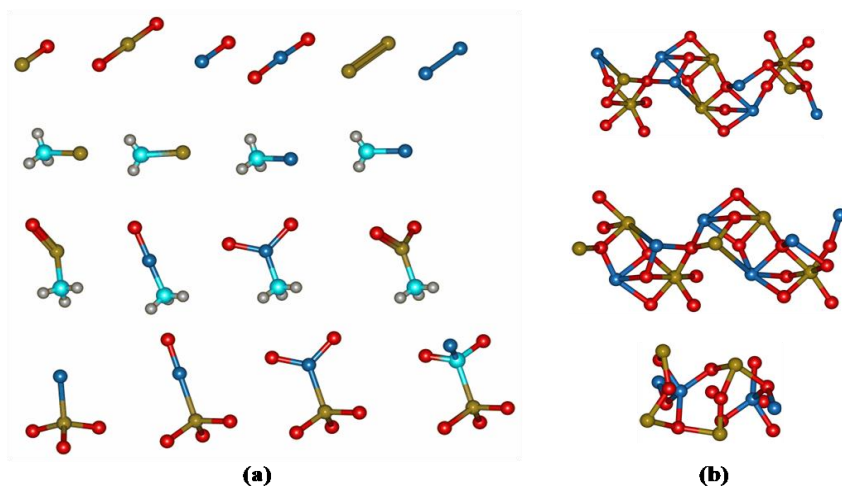


PP=14 (56%)





**Figure S1.** Models of 20 different ZS/PP composites with various ratios for combustions.



**Figure S2.** Structures of partial training set. **(a)** Scanning of different bonds, angles, and transition states; **(b)** Scanning of ZS crystals with different space groups.