

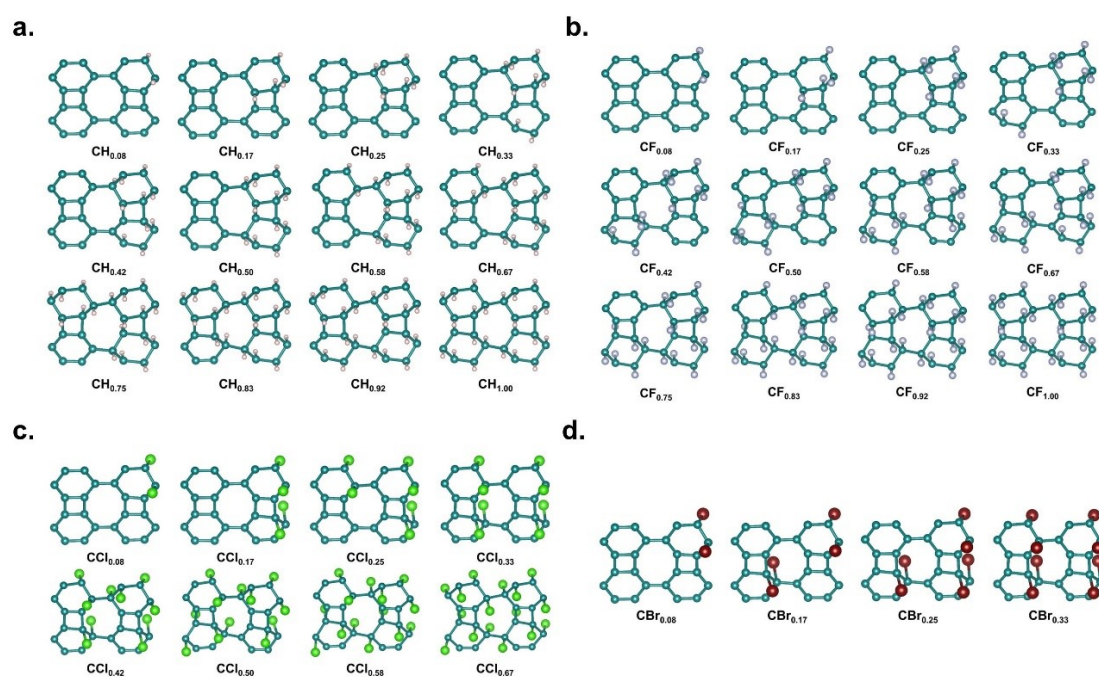
# Effective regulation of the electronic properties of biphenylene network by hydrogenation and halogenation

Yunhao Xie,<sup>a</sup> Liang Chen,<sup>a,b</sup> Jing Xu,<sup>a,\*</sup> Wei Liu<sup>a,\*</sup>

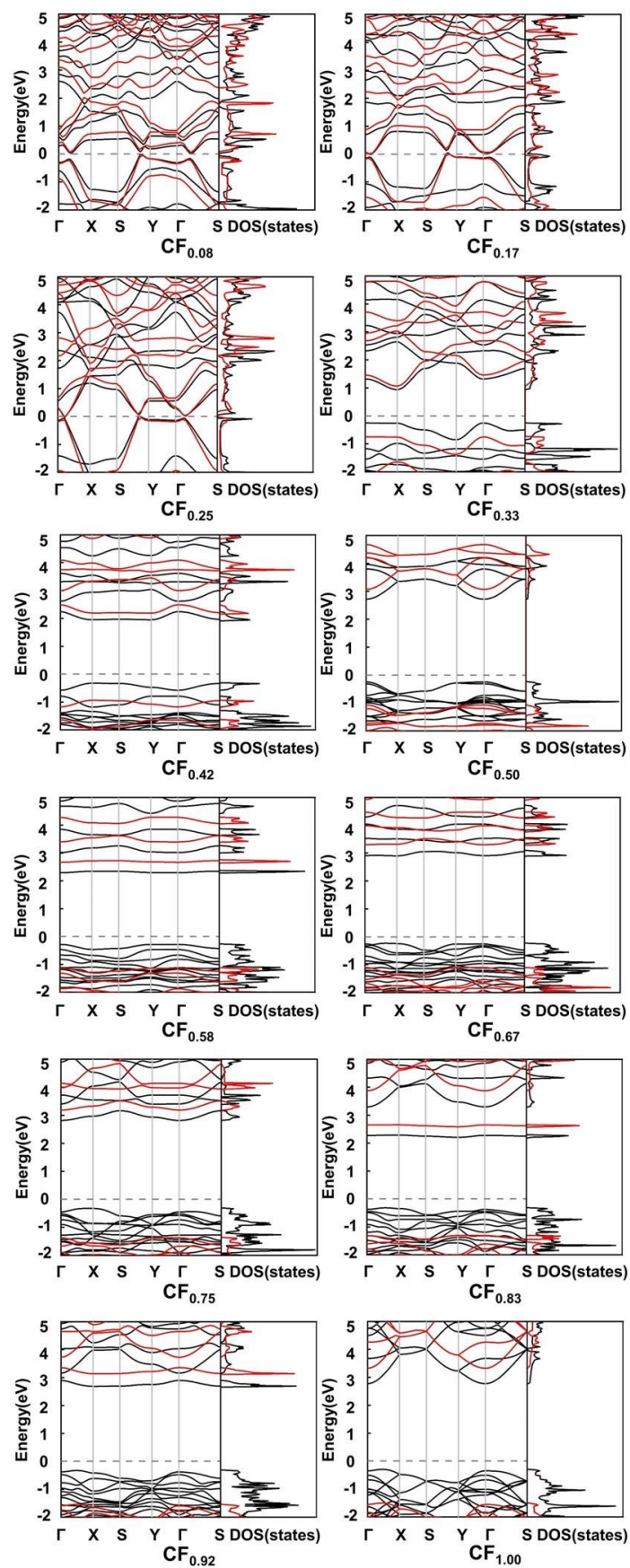
<sup>a</sup> Department of Optical Engineering, College of Optical, Mechanical and Electrical Engineering, Zhejiang A&F University, Hangzhou, Zhejiang, 311300, P. R. China

<sup>b</sup> School of Physical Science and Technology, Ningbo University, Ningbo, Zhejiang, 315211, P. R. China

Email: weiliu@zafu.edu.cn; [jingxu@zafu.edu.cn](mailto:jingxu@zafu.edu.cn)



**Fig. S1** The top views of structures of biphenylene networks functionalized by H (a), F (b), Cl (c) and Br (d) at different concentrations.



**Fig. S2** The PBE (black lines) and HSE (red lines) band structures of fluorinated biphenylenes at different fluorine concentration  $x$ . The Fermi levels are shown by dashed lines.

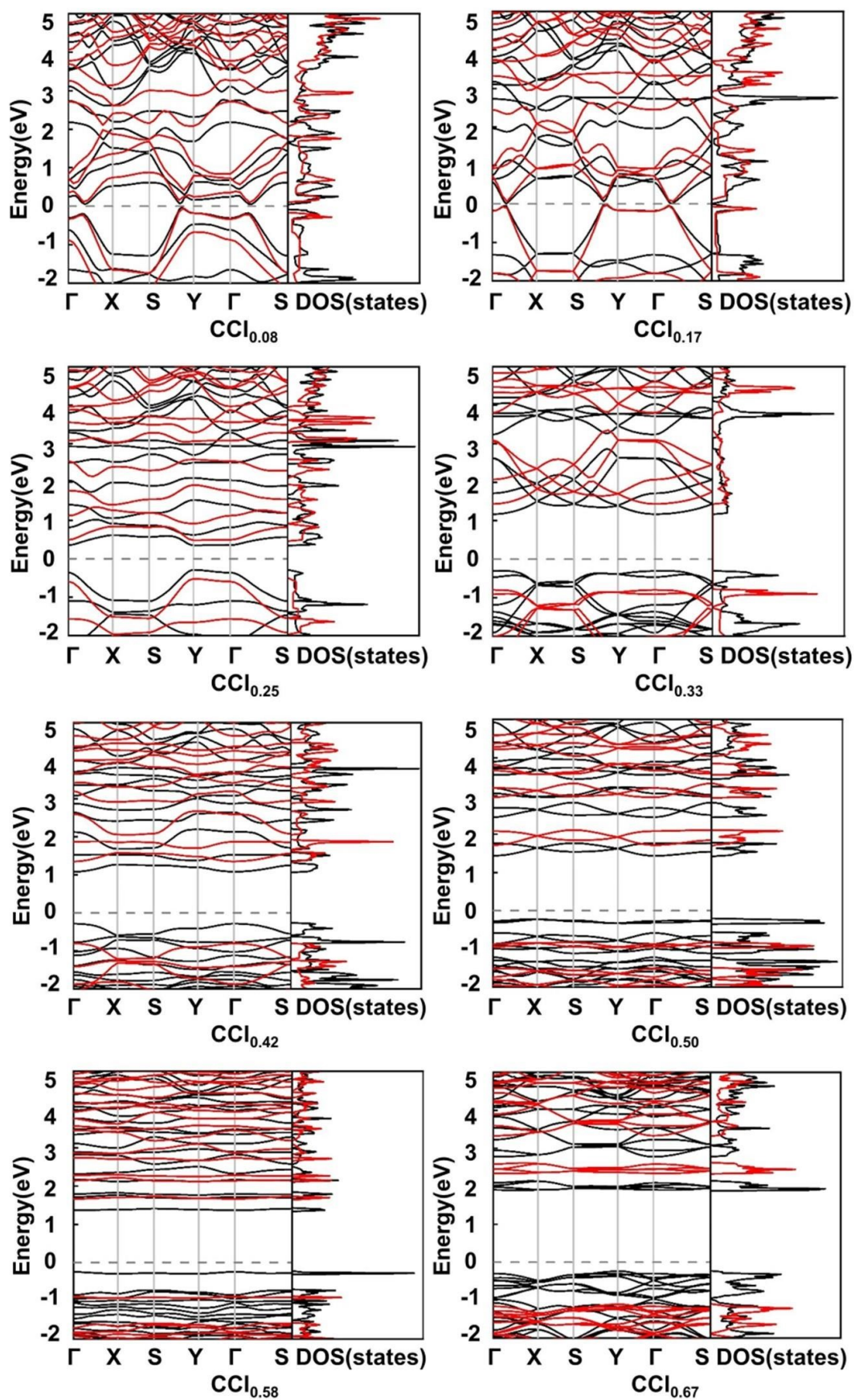
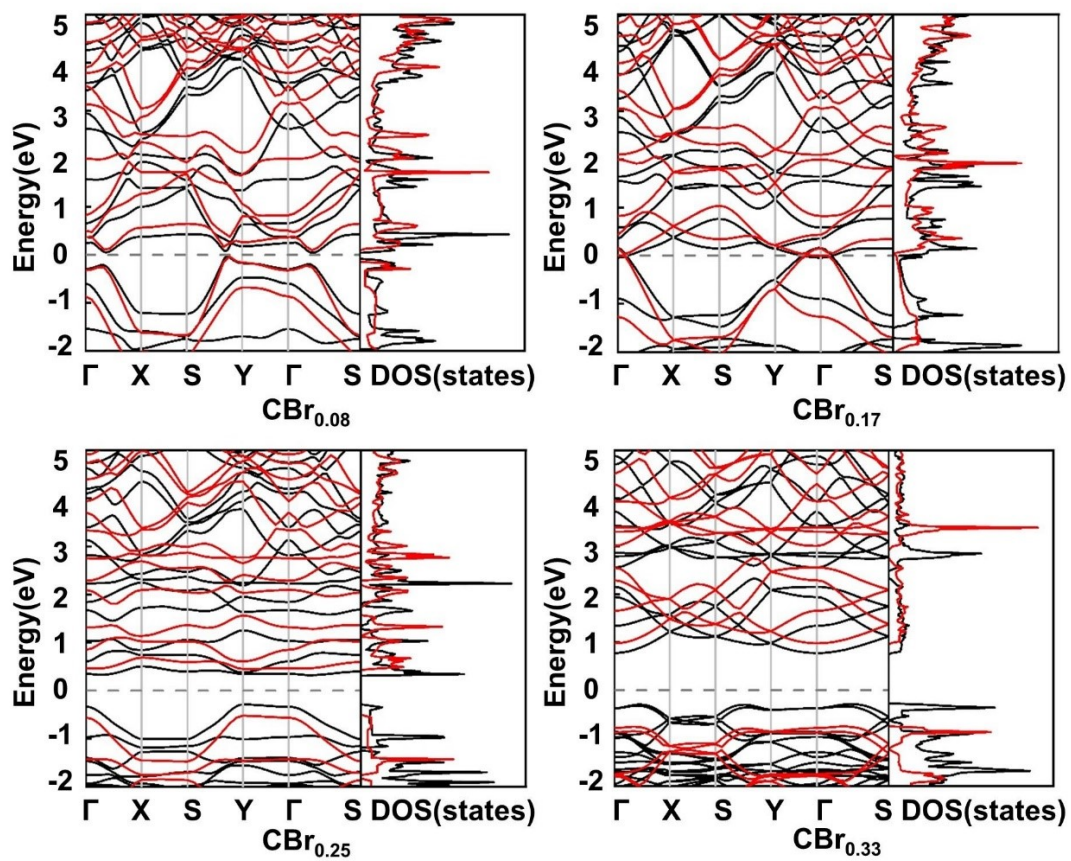


Fig. S3 The PBE (black lines) and HSE (red lines) band structures of chlorinated biphenylenes at different chlorine concentration  $x$ . The Fermi levels are shown by dashed lines.



**Fig. S4** The PBE (black lines) and HSE (red lines) band structures of brominated biphenylenes at different bromine concentration  $x$ . The Fermi levels are shown by dashed lines.