

Supporting Information

Electronic and optical properties of hydrogen-terminated biphenylene nanoribbon : a first-principles study

Hong Shen¹, Riyi Yang¹, Kun Xie¹, Zhiyuan Yu¹, Yuxiang Zheng¹, Rongjun Zhang¹, Liangyao Chen¹, Bi-Ru Wu² and Wan-Sheng Su^{3,4,*}, Songyou Wang^{1,5,6,*}

¹Shanghai Ultra-Precision Optical Manufacturing Engineering Center, Department of Optical Science and Engineering, Fudan University, Shanghai 200433, China

²Division of Natural Science, Center for General Education, Chang Gung University, Tao-Yuan 33302, Taiwan

³National Taiwan Science Education Center, Taipei 11165, Taiwan.

⁴Department of Electro-Optical Engineering, National Taipei University of Technology, Taipei 10608, Taiwan

⁵Key Laboratory for Information Science of Electromagnetic Waves (MoE), Shanghai 200433, China

⁶Yiwu Research Institution of Fudan University, Yiwu 322000, China

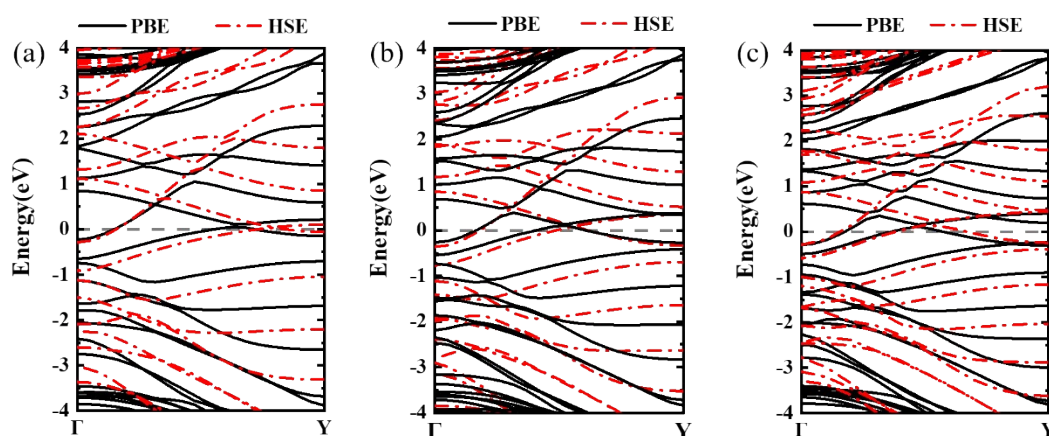


Figure S1. Band structures of nanoribbons with widths of (a) 15-ABNR, (b) 18-ABNR, and (c) 21-ABNR. The PBE and HSE06 band structures are represented by solid and dashed lines, respectively.

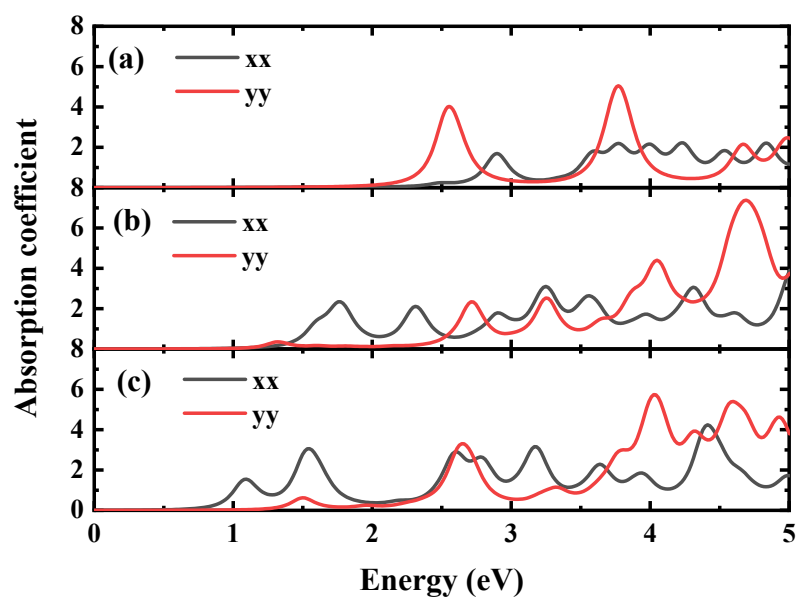


Figure S2. The x and y component of the absorption coefficients of (a) 6-ABNR, (b) 9-ABNR and (c) 12-ABNR.