Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Materials

First-principles calculation of the optical properties of the $YBa_2Cu_3O_{7-\delta}$ oxygen vacancy model

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S1. Planar and apical vacancy models

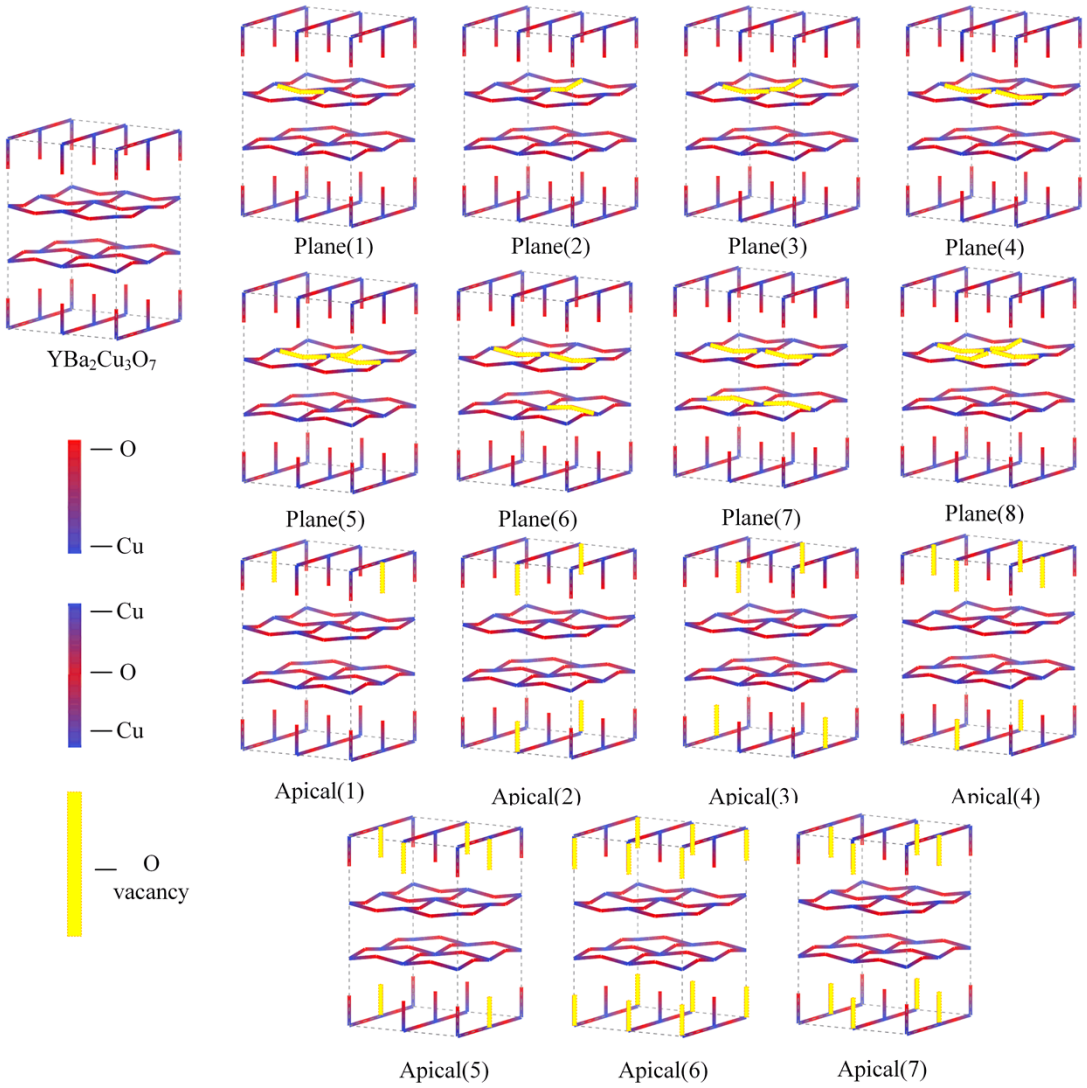

Figure S1 The planar and apical vacancy models of $YBa_2Cu_3O_{7-\delta}$. The blue bars represent Cu, the red bars represent O, and the blue and red bars represent a Cu-O bond. Yellow bars represent the positions of oxygen vacancies.

S2. Energy band calculation results for YBCO and its oxygen vacancy model

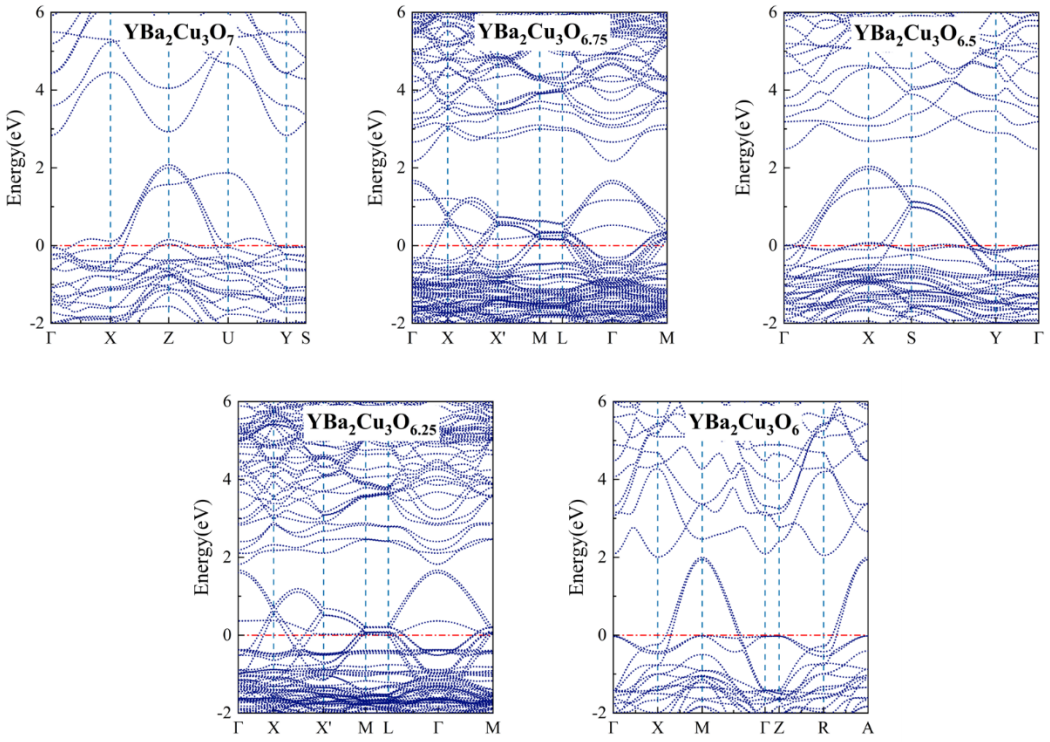

Figure S2 Band structure results of YBCO and its vacancy models. (a) δ=0 $YBa_2Cu_3O_7$ (b) δ=0.25 $YBa_2Cu_3O_{6.75}$ (c) δ=0.5 $YBa_2Cu_3O_{6.5}$ (d) δ=0.75 $YBa_2Cu_3O_{6.25}$ (e) δ=1 $YBa_2Cu_3O_6$.

S3. The optical absorption spectrum of $YBa_2Cu_3O_{6.25}$ calculated with PBE and PBE+U

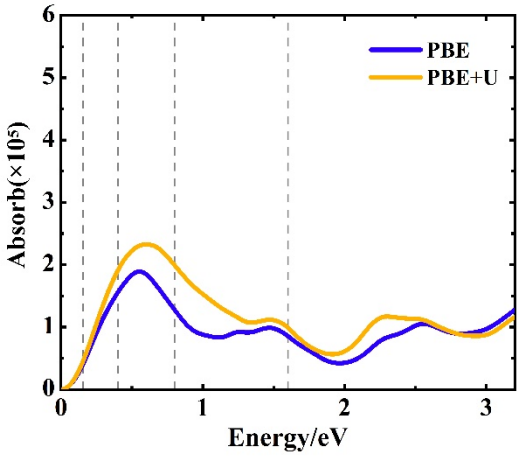

Figure S3 The optical absorption spectrum of $YBa_2Cu_3O_{6.25}$ in the a-direction calculated with PBE and PBE+U (U-J=9eV, applied with the d-orbital of Cu atom). The blue represents the calculation results using the PBE method, and the yellow represents the PBE+U method