

$G_0W_0@PBEh(\alpha = 0.45)$ 

O 1s Binding Energy [eV]

535  
536  
537  
538  
539  
540

w1  
w2  
w3  
w4  
w5  
w5\_solvated  
w6\_cage  
w6\_book  
w6\_prism  
w6\_ring  
w8\_cube  
w8\_d2d  
w8\_solvated  
w10\_1  
w10\_2  
w10\_3  
w10\_4  
w10\_5  
w11  
w13\_127  
w13\_128  
w17\_6076  
w17\_6711  
w17\_6759  
w17\_solvated  
w18  
w20\_cage  
w20\_dodecahedron  
w20\_edge  
w20\_face  
w20\_fused

