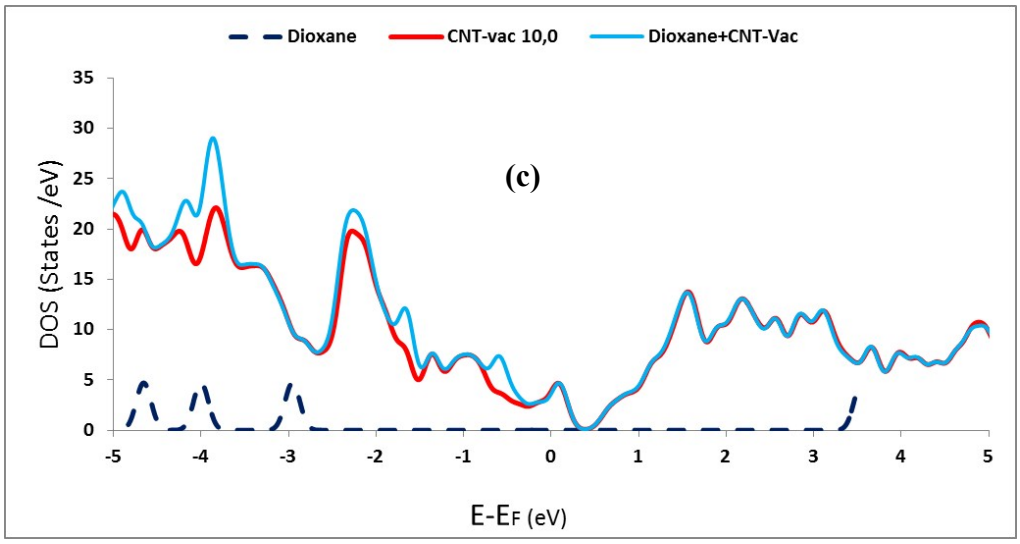
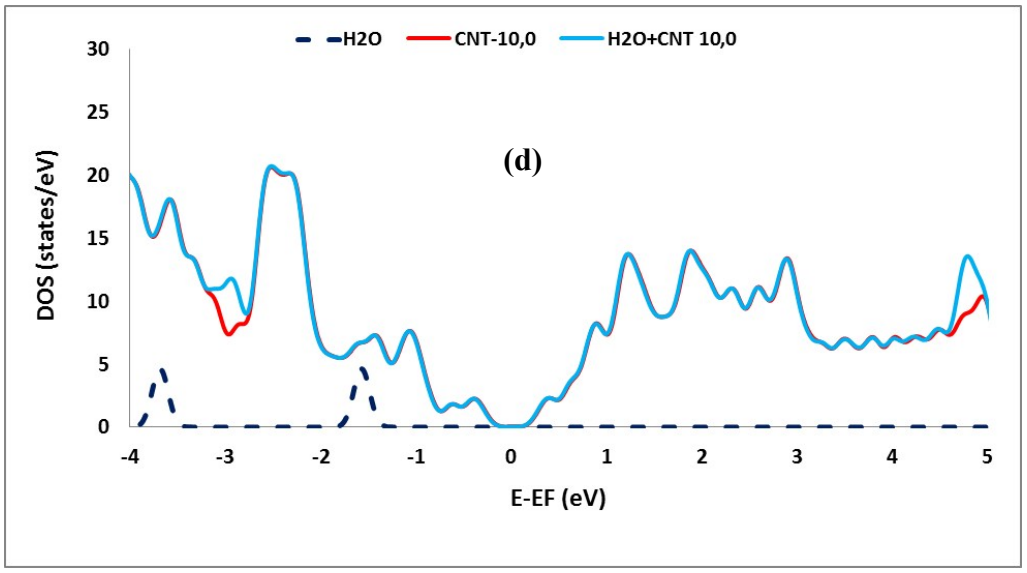
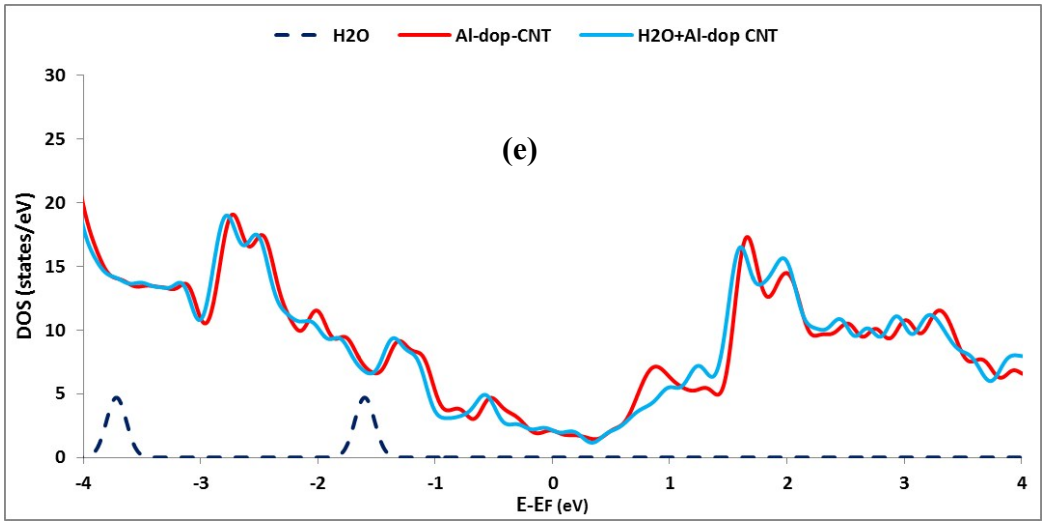
Figure 5: Comparison between the density of states (DOS) for an isolated dioxane molecule, an isolated CNT (10, 0), and the combination of the two at equilibrium geometry for energetically favorable (c) dioxane/CNT (10, 0) with defect systems and, (d) H_2O/CNT (10, 0), and (e) H_2O/Al-CNT (10, 0).






H2O
Al-dop-CNT
H2O+Al-dop CNT
(e)
DOS (states/eV)
E-EF (eV)
30
25
20
15
10
5
0
-4
-3
-2
-1
0
1
2
3
4