Supporting data

Exploring the performance of pristine and vacancy defected $B_3C_2N_3$ nanosheets for detecting and removal of environmentally harmful radicals: A DFT study

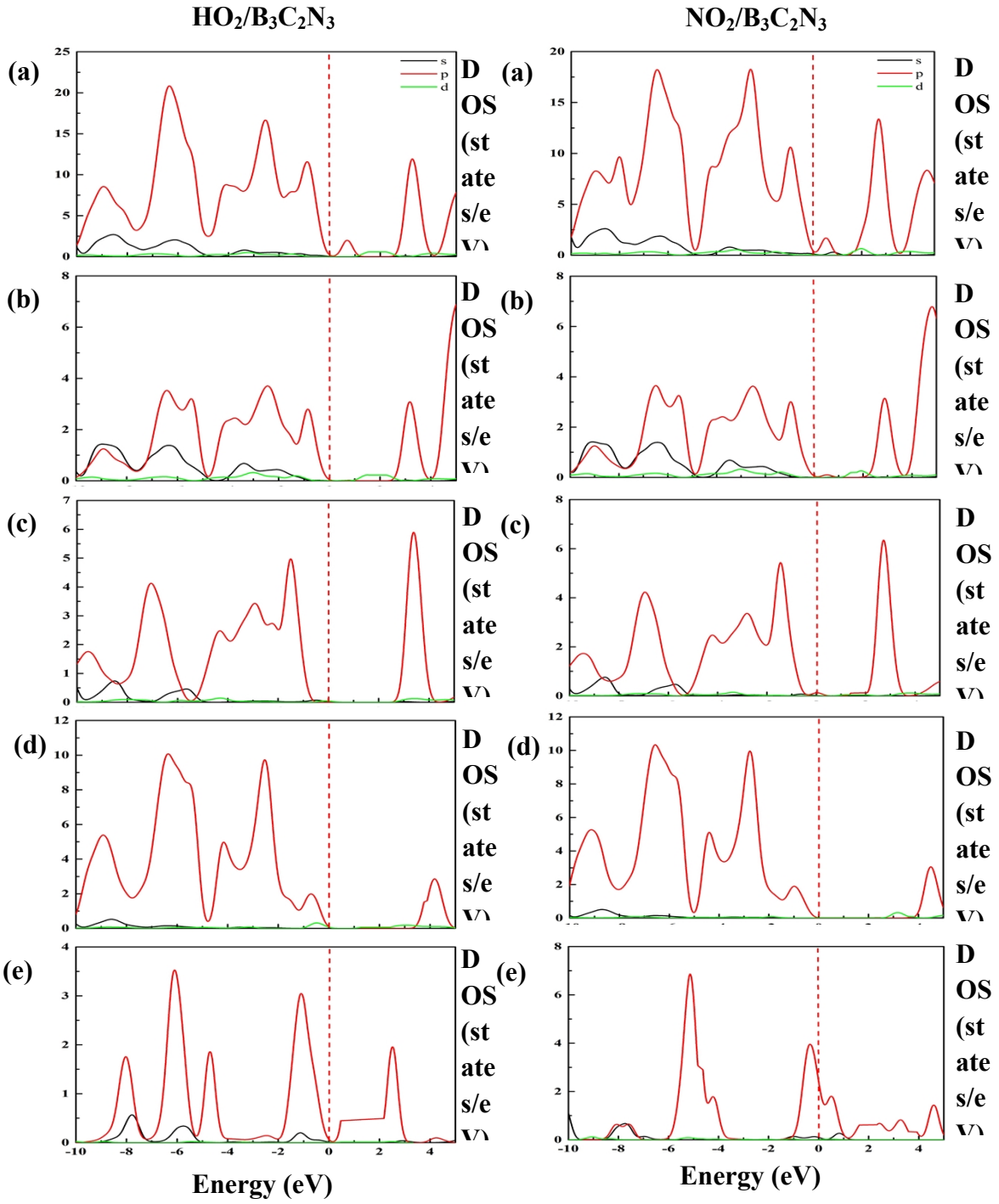
Rezvan Rahimi *[a, b], Mohammad Solimannejad*[a, b]

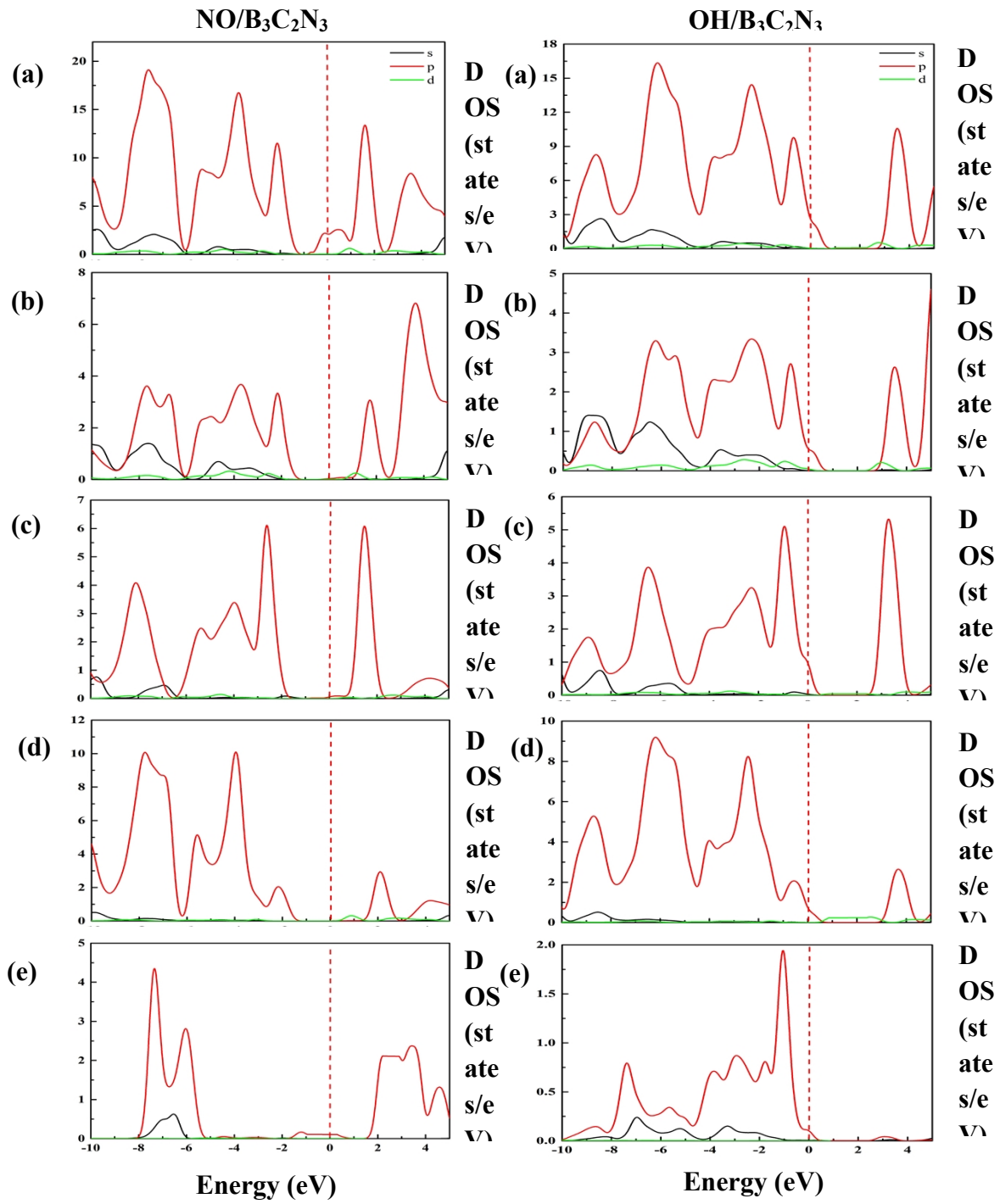
[a] Department of Chemistry, Faculty of Science, Arak University, Arak 3848177584, Iran

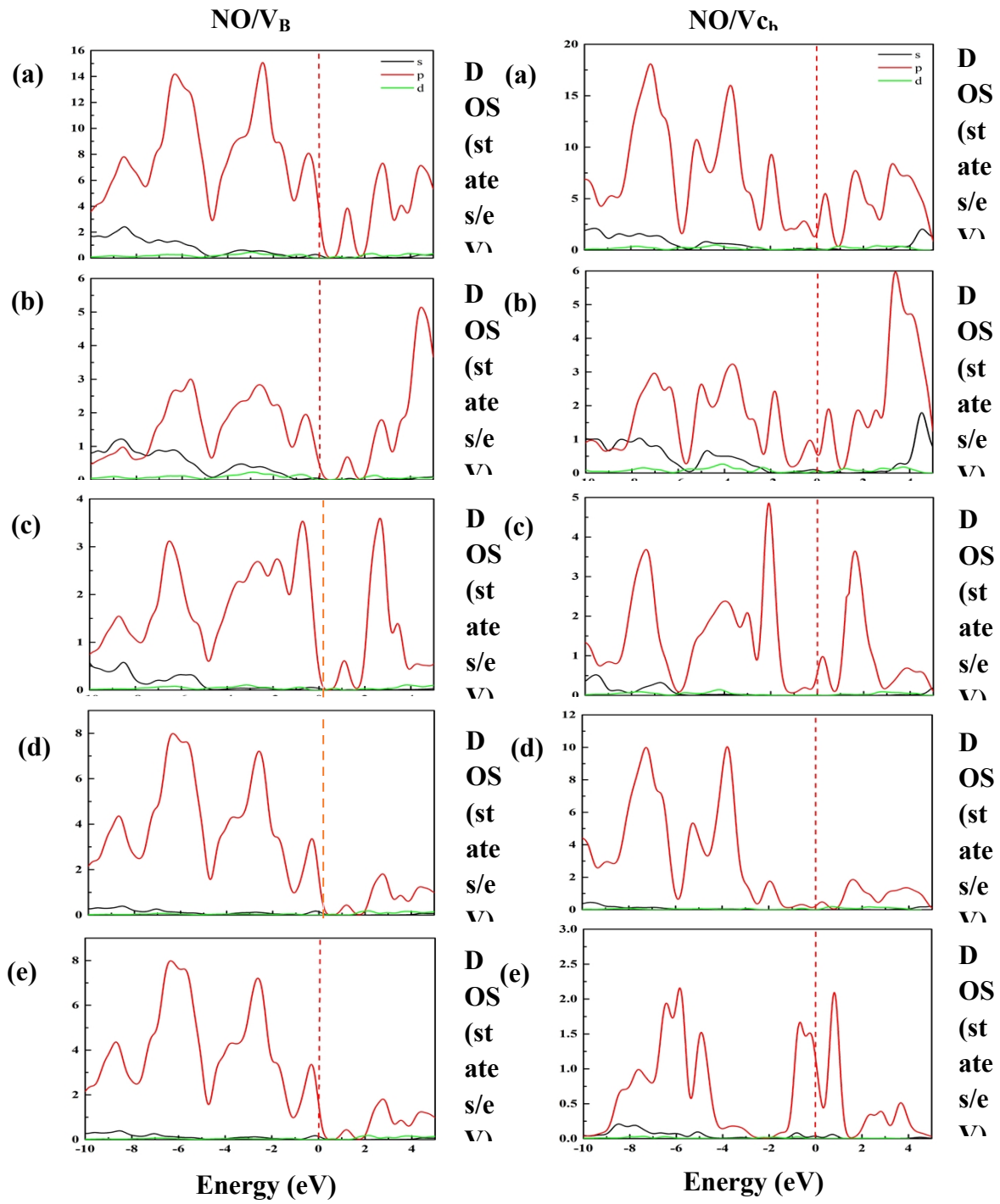
[b] Institute of Nanosciences and Nanotechnology, Arak University, Arak, Iran

* Corresponding authors:

r.rahimi1989@gmail.com (R. Rahimi), m-solimannejad@araku.ac.ir (M. Solimannejad)


HO2/B3C2N3
NO2/B3C2N3
(a)
(b)
(c)
(d)
(e)
s
p
d
DOS (state s/eV)
Energy (eV)


NO/B3C2N3
OH/B3C2N3
(a)
(b)
(c)
(d)
(e)
s
p
d
DOS (state s/eV)
Energy (eV)


NO/V_B
NO/Vc_h
(a)
(b)
(c)
(d)
(e)
s
p
d
DOS (state s/eV)
Energy (eV)

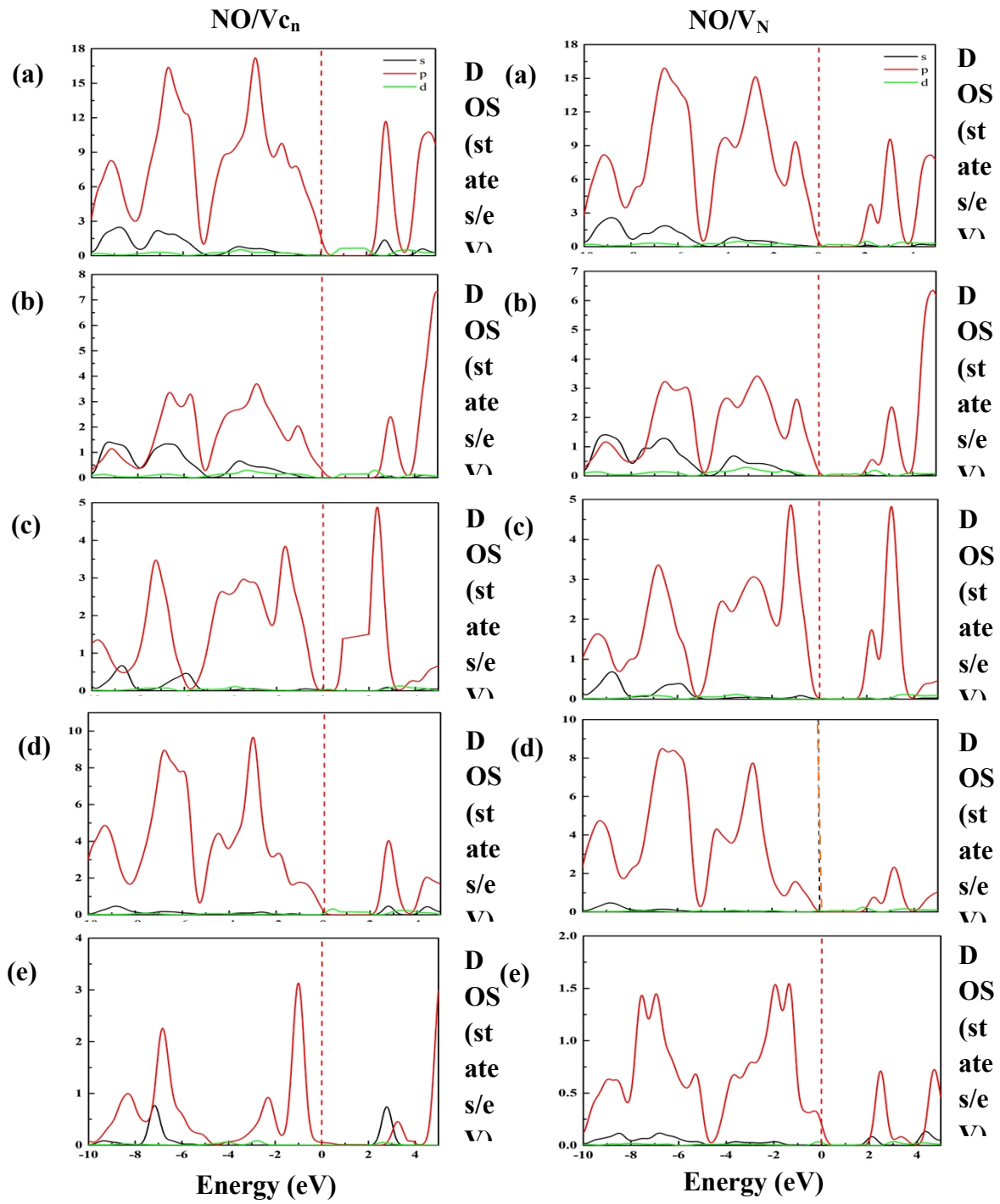
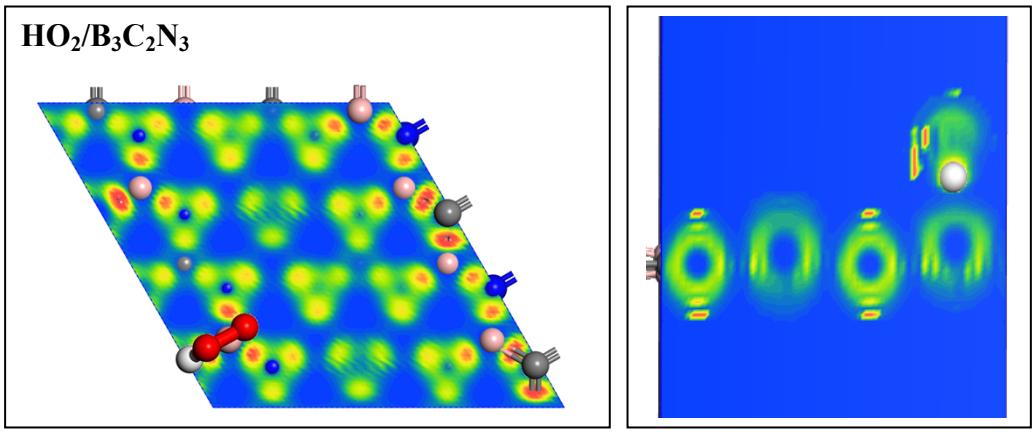
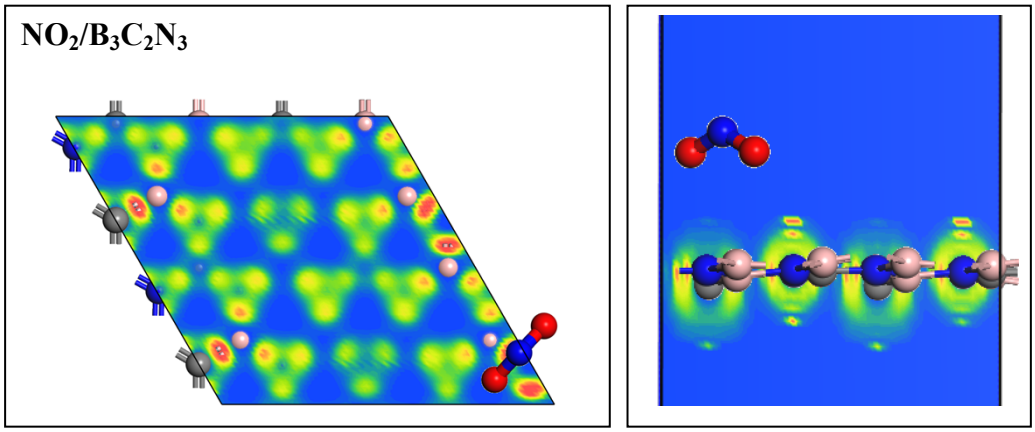


Figure S1. Partial density of state plots for the pristine and vacancy defect $B_3C_2N_3$ after the adsorption of the radical molecules. The (a) radical/pristine and vacancy defect $B_3C_2N_3$ complexes, (b) B atom in complex, (c) C atom in complex, (d) N atom in complex, (e) radical molecule in complex. The dark red dotted line indicates the position of the Fermi level at zero eV. The black, red, and green curves represent the *s*, *p*, and *d* orbitals, respectively.

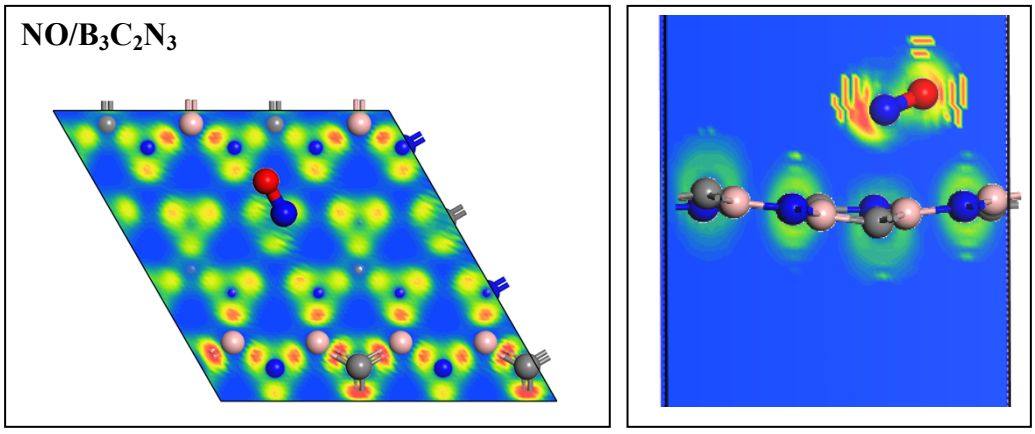
(a)



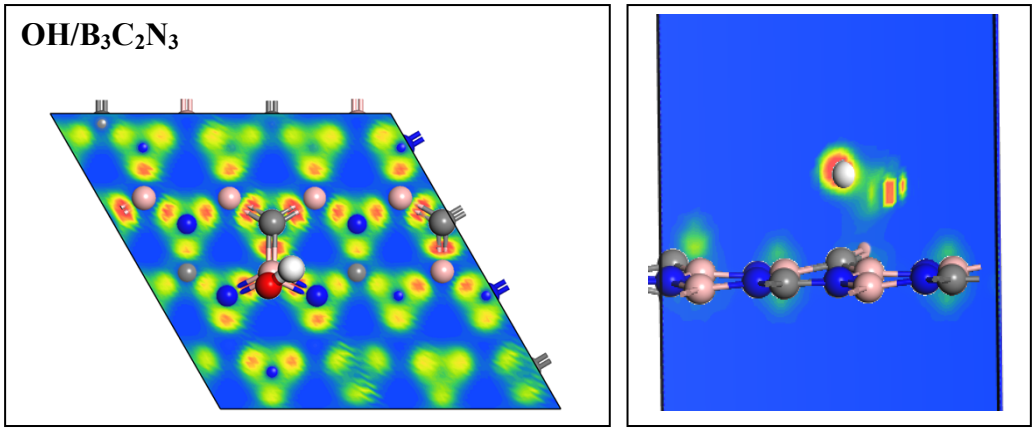
(b)



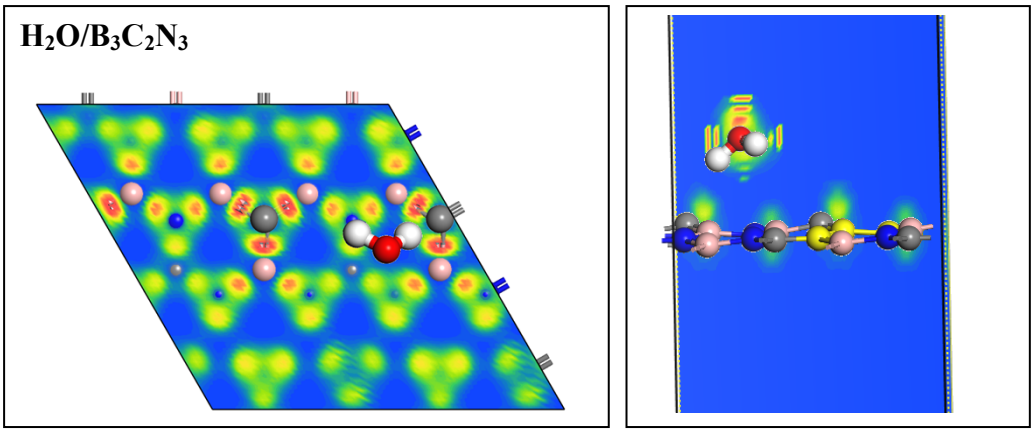
(c)



(d)



(e)



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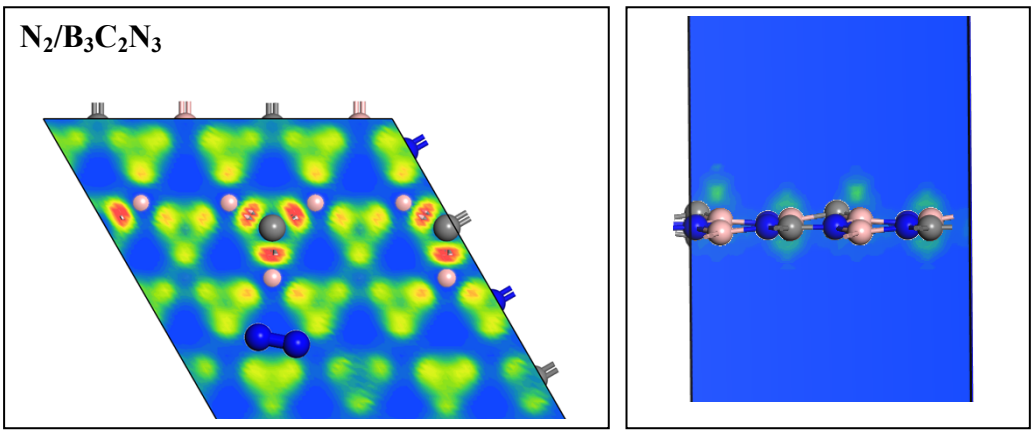
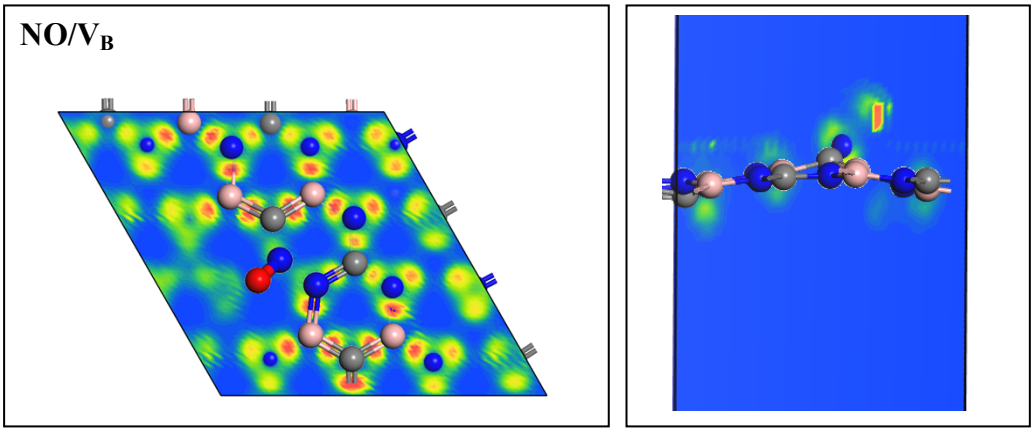
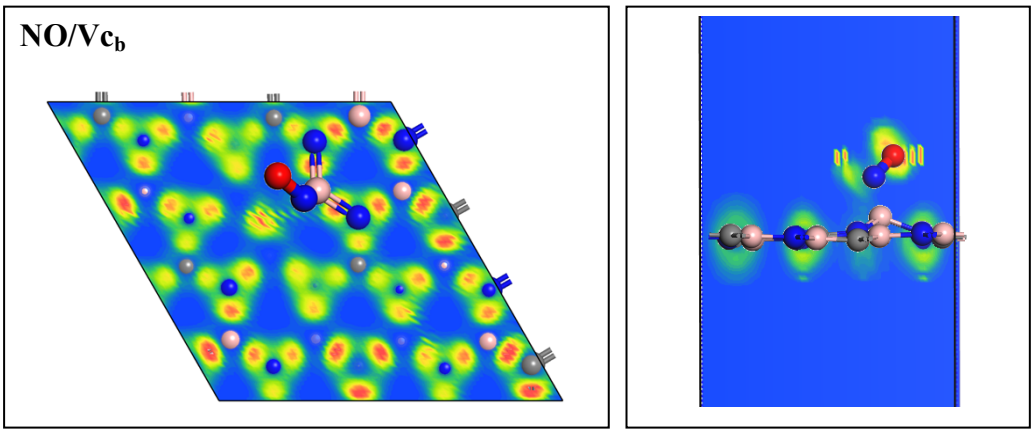


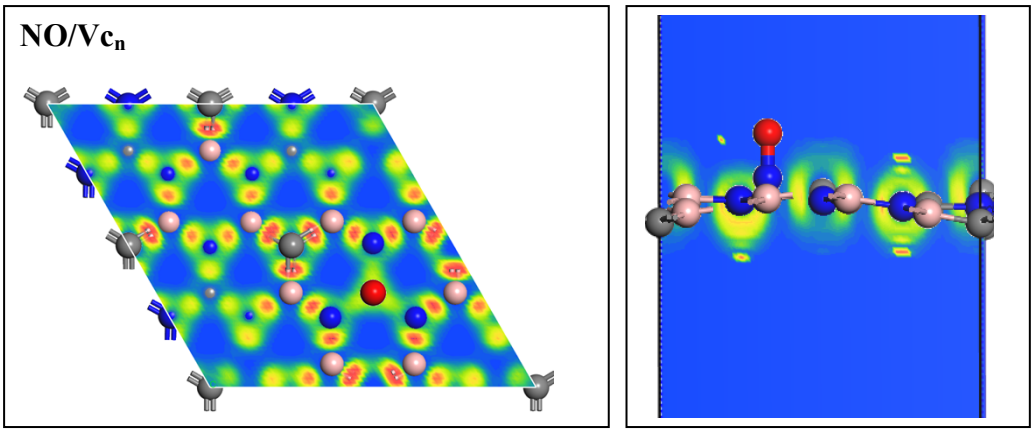
(g)



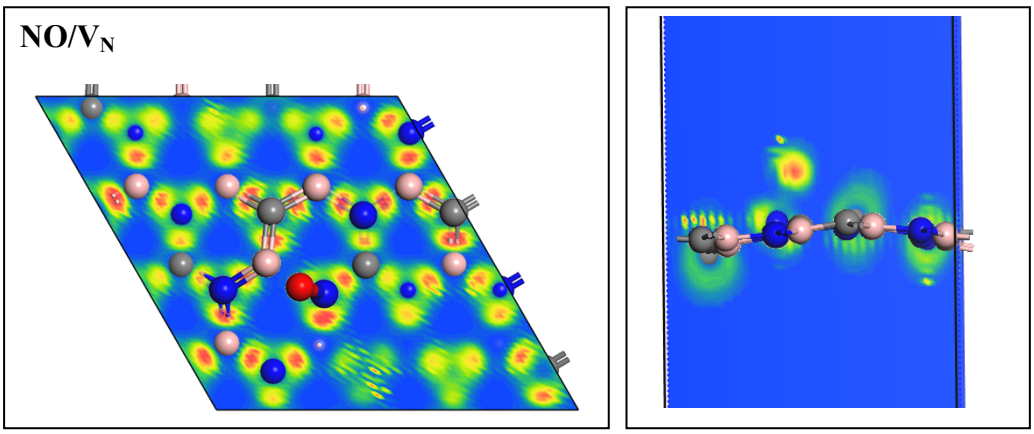
(h)



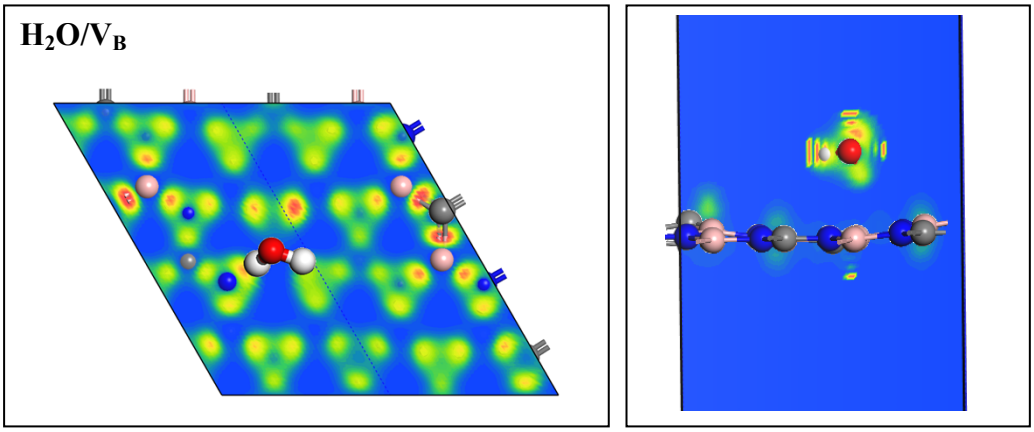
(i)



(j)



(k)



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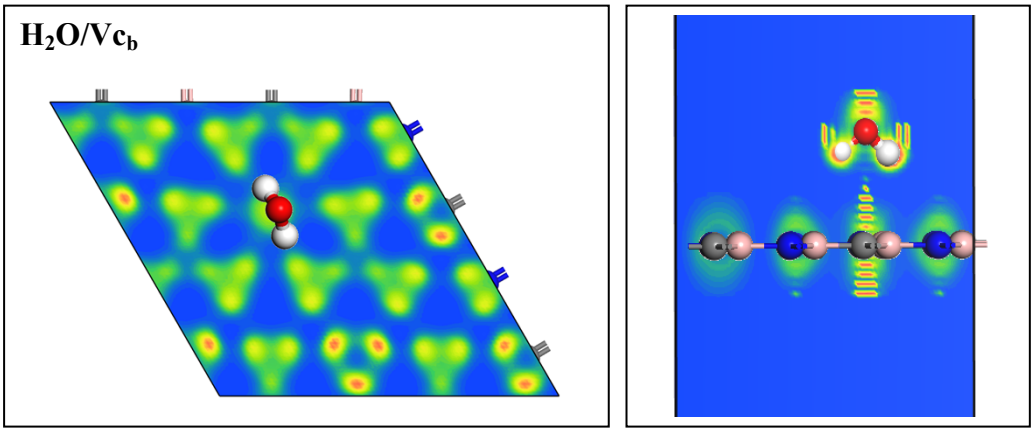
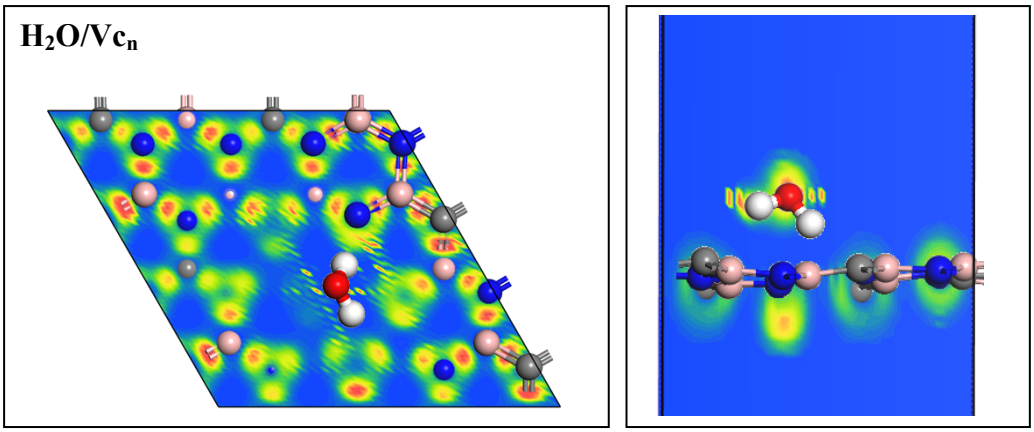
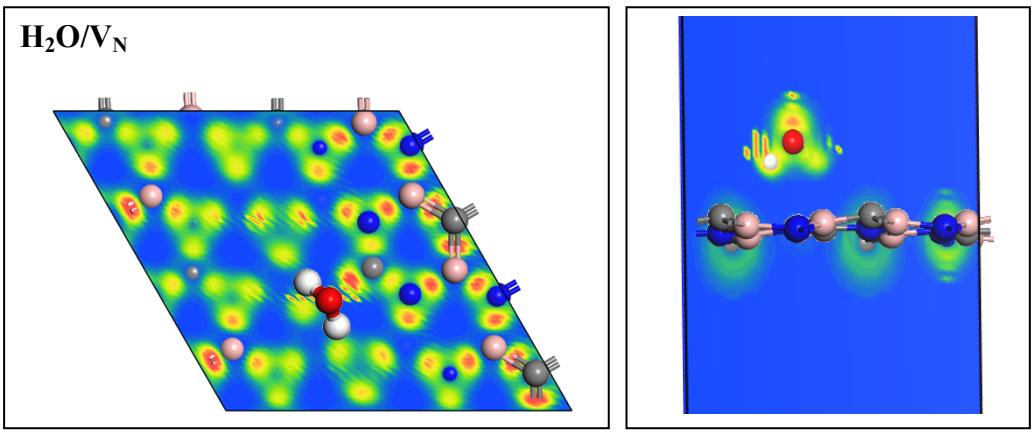


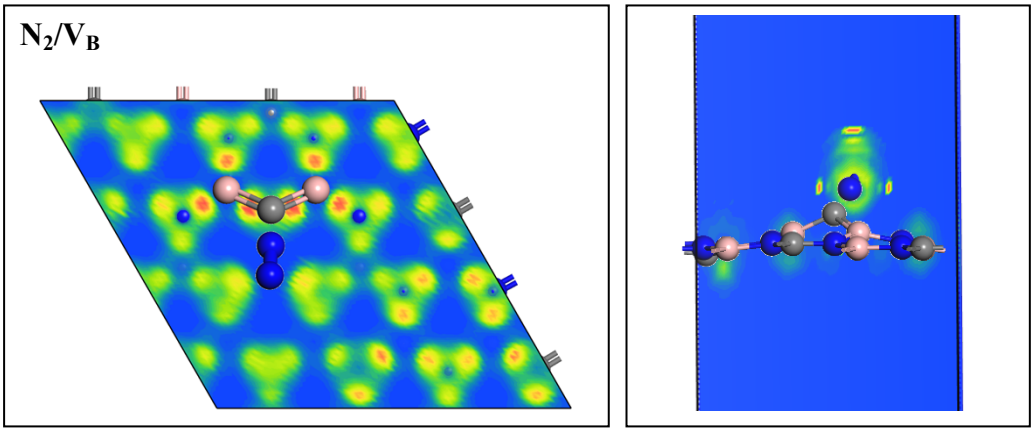
(m)



(n)



(o)



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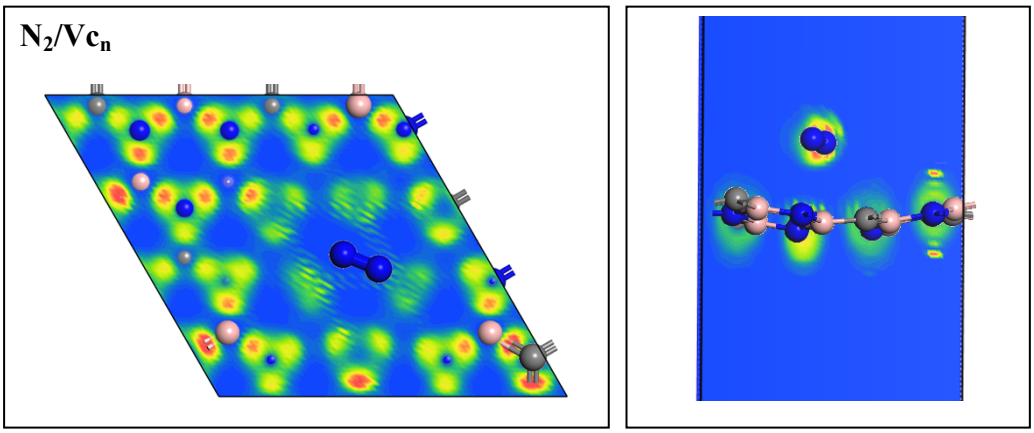

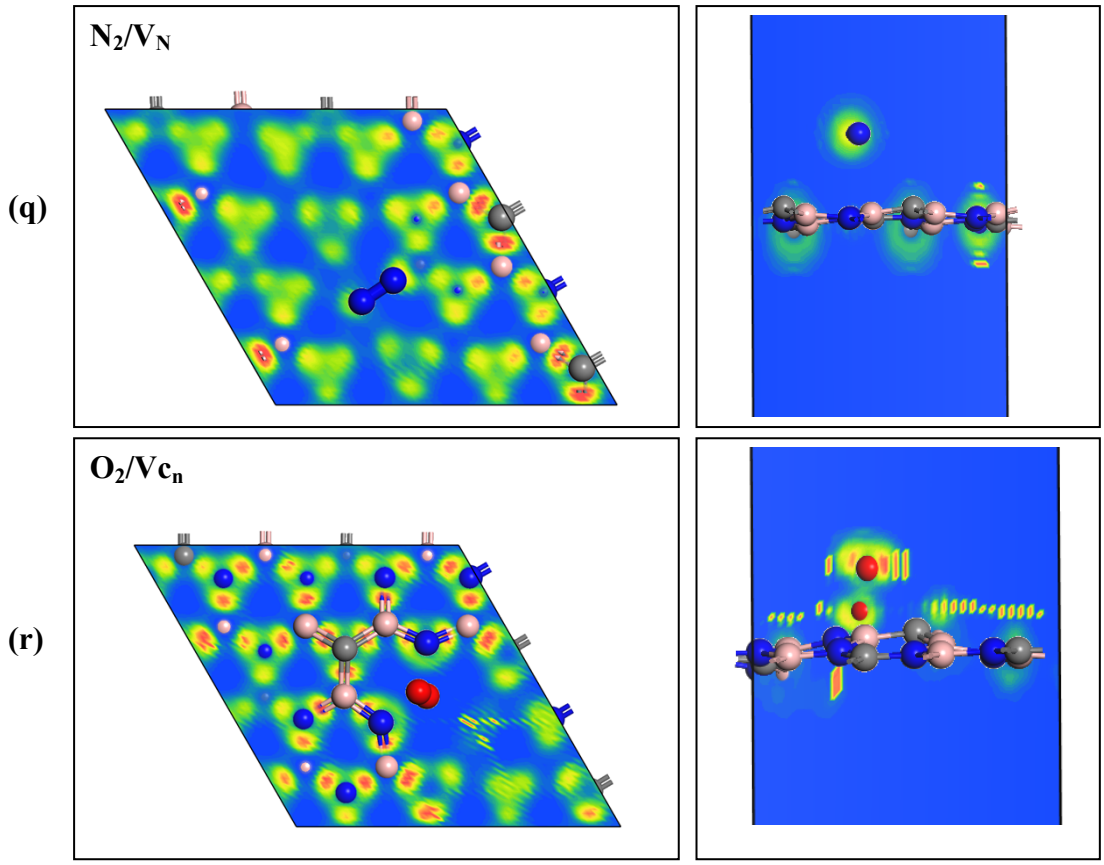

Figure S2. (a-r) The electron localization function (ELF) scheme for the most stable configurations of radicals and interfering species adsorbed on pristine and vacancy defect $B_3C_2N_3$ monolayer. The ELF values (0 to 1) have plotted on a red-green-blue color scale.