Supporting information file

Quantum Design of Transition Metals Decorated on Boron Phosphide Inorganic Nanocluster for Favipiravir Adsorption: A Possible Treatment for Covid-19

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Table S1: Spin state of all studied systems.

System	Spin state
F@ $B_{12}P_{12}$	Singlet
Sc-$B_{12}P_{12}$	Singlet
F@Sc-$B_{12}P_{12}$	Doublet
Ti-$B_{12}P_{12}$	Singlet
F@Ti-$B_{12}P_{12}$	Doublet
V-$B_{12}P_{12}$	Doublet
F@V-$B_{12}P_{12}$	Singlet
Cr-$B_{12}P_{12}$	Doublet
F@Cr-$B_{12}P_{12}$	Doublet
Mn-$B_{12}P_{12}$	Singlet
F@Mn-$B_{12}P_{12}$	Singlet
Fe-$B_{12}P_{12}$	Doublet
F@Fe-$B_{12}P_{12}$	Singlet
Co-$B_{12}P_{12}$	Singlet
F@Co-$B_{12}P_{12}$	Singlet
Ni-$B_{12}P_{12}$	Doublet
F@Ni-$B_{12}P_{12}$	Singlet
Cu-$B_{12}P_{12}$	Doublet
F@Cu-$B_{12}P_{12}$	Doublet
Zn-$B_{12}P_{12}$	Doublet
F@Zn-$B_{12}P_{12}$	Singlet

Table S1 expressed the spin states of the studied systems. From table, it is clearly indicated that studied systems are quite stable in singlet and doublet state. Furthermore, no imaginary frequency is noted for studied systems which suggested that studied systems are at true global minima.