

Supplementary Information

Adsorption of Thymine and Uracil on 1:1 Clay Mineral Surfaces: Comprehensive *ab initio* study on Influence of Sodium Cation and Water

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Figure captions:

Figure 1. The structures of small models of six member rings of the siloxane (A-D) and octahedral sheet (E and F) of the mineral of the kaolinite group used in this study.

Figure 2. The optimized structure of thymine adsorbed on non-hydrated tetrahedral surface of kaolinite mineral (all stable positions) obtained at the B3LYP/6-31G(d) level of theory.

Figure 3. The optimized structure of thymine adsorbed on non-hydrated octahedral surface of kaolinite mineral (all stable positions) obtained at the B3LYP/6-31G(d) level of theory.

Figure 4. The optimized structure of uracil adsorbed on hydrated tetrahedral surface of kaolinite mineral (all stable positions) obtained at the B3LYP/6-31G(d) level of theory.

Figure 5. The optimized structure of thymine adsorbed on hydrated tetrahedral surface of kaolinite mineral (all stable positions) obtained at the B3LYP/6-31G(d) level of theory.

Figure 6. The optimized structure of uracil adsorbed on hydrated octahedral surface of kaolinite mineral (all stable positions) obtained at the B3LYP/6-31G(d) level of theory.

Figure 7. The optimized structure of thymine adsorbed on hydrated octahedral surface of kaolinite mineral (all stable positions) obtained at the B3LYP/6-31G(d) level of theory.

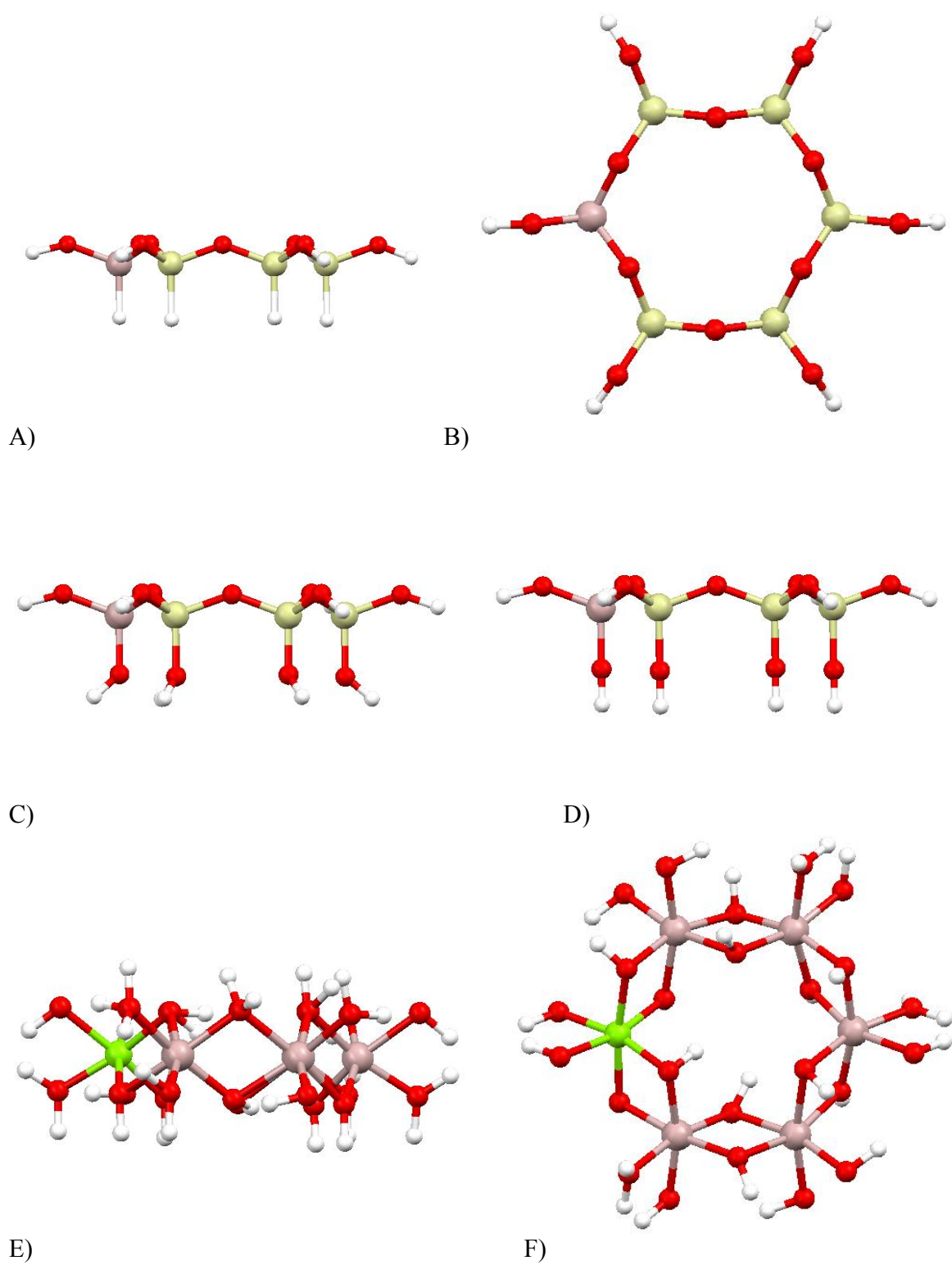
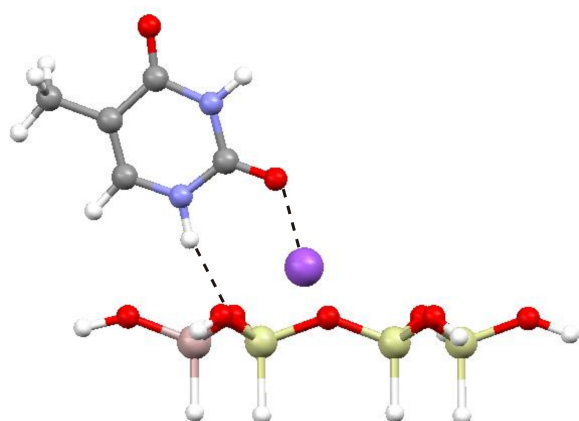
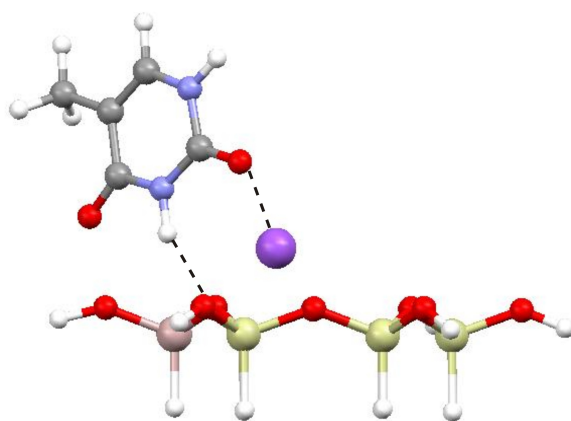


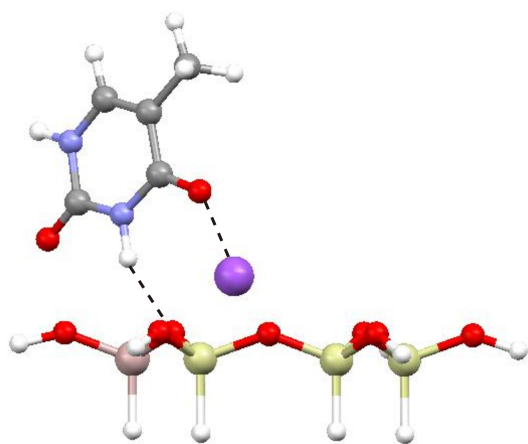
Figure 1.



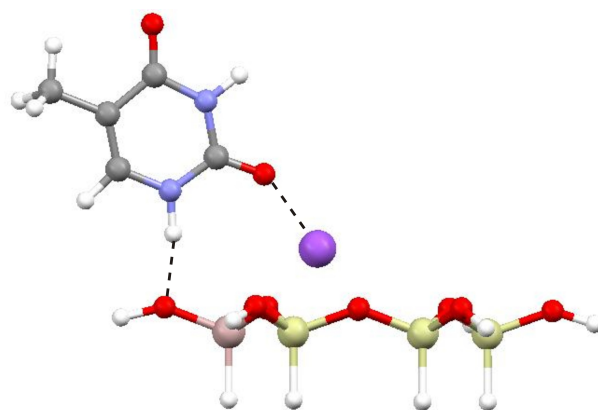
A) Na-O2(O4top)



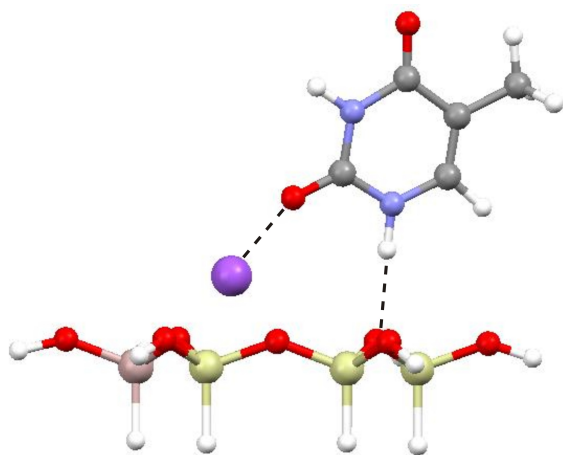
B) Na-O2



C) Na-O4



D) Na-O2(O4top)side



E) Na-O2-r

Figure 2.

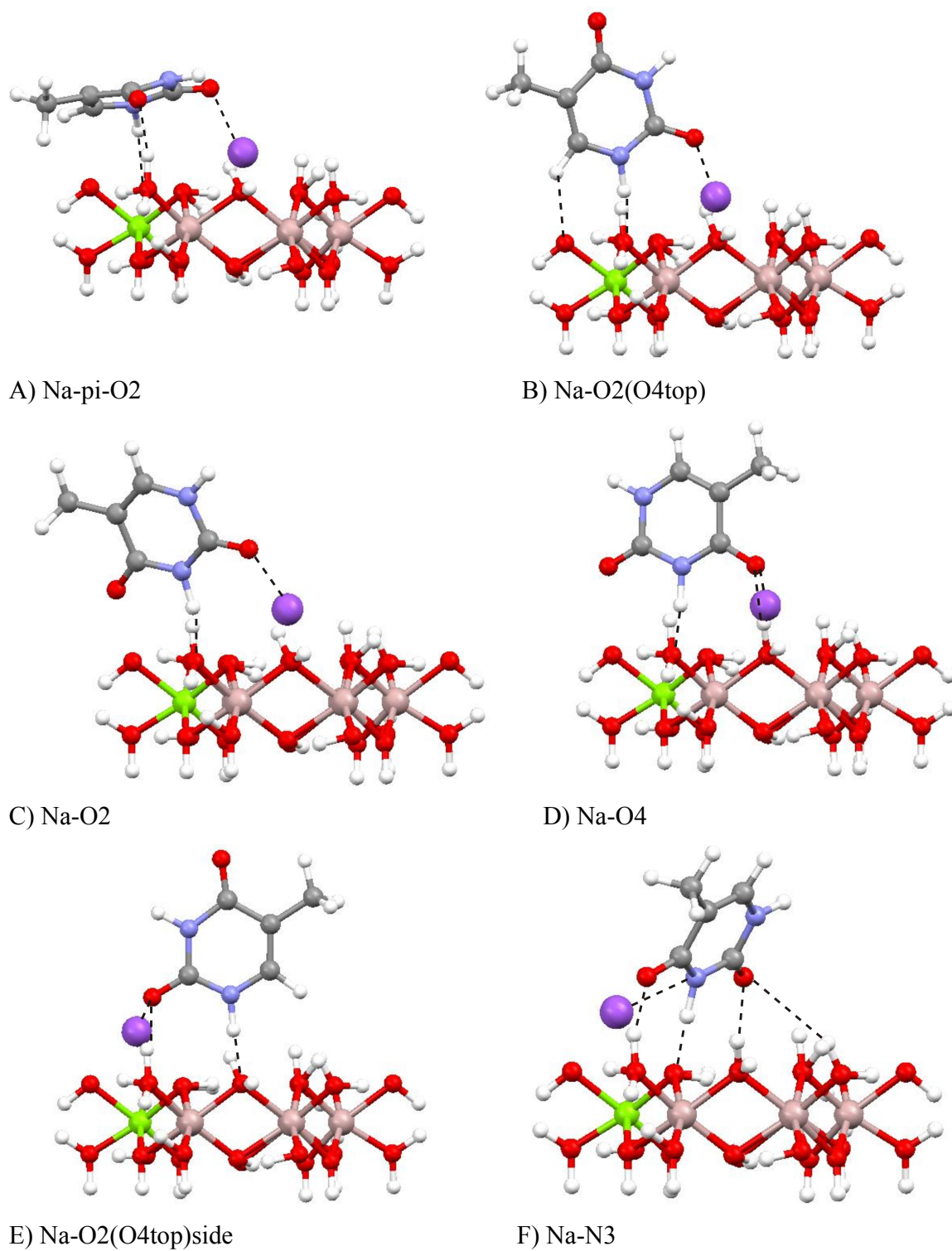
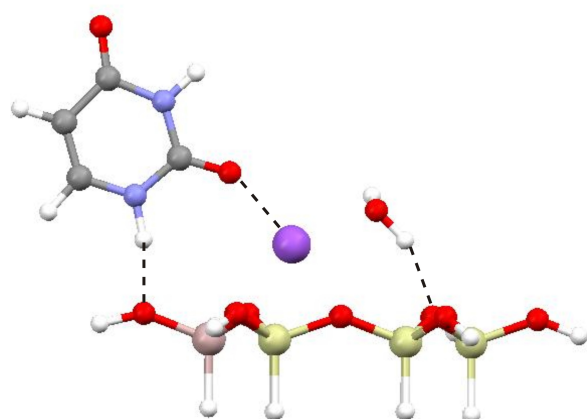
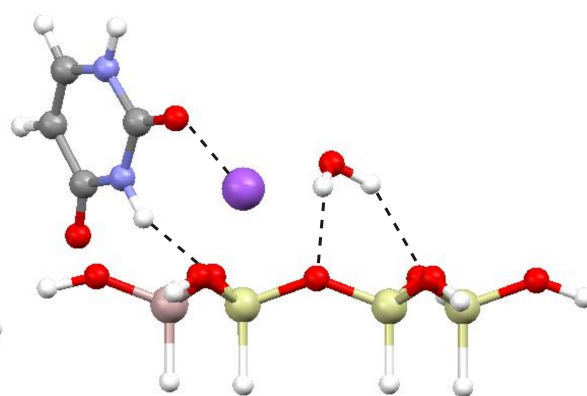


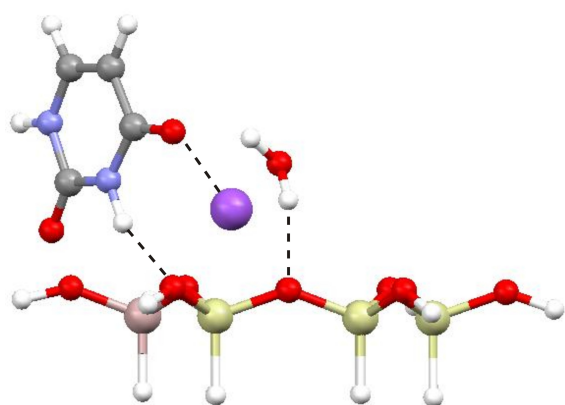
Figure 3.



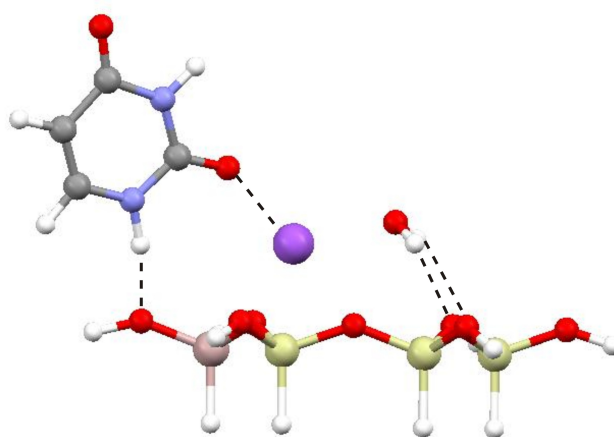
A) Na-O2(O4top)



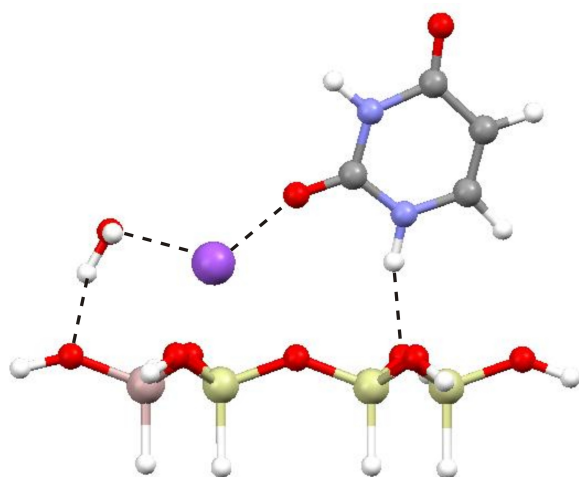
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C) Na-O4

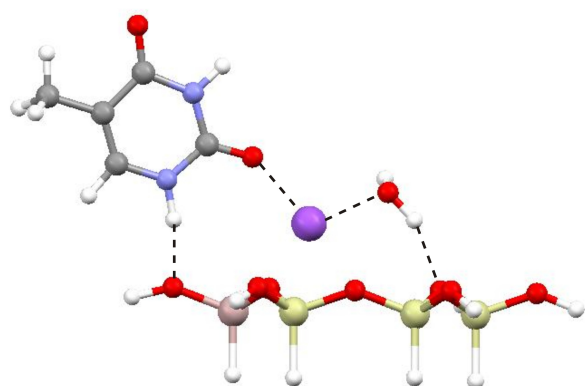


D) Na-O2(O4top)side

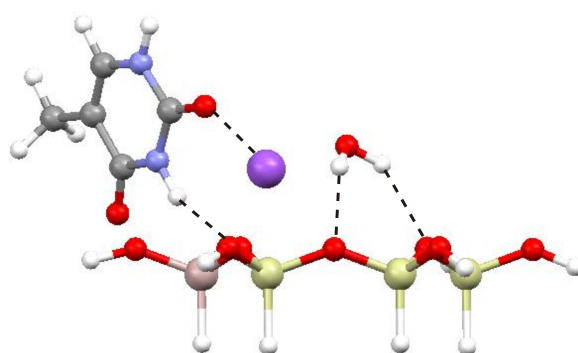


E) Na-O2-r

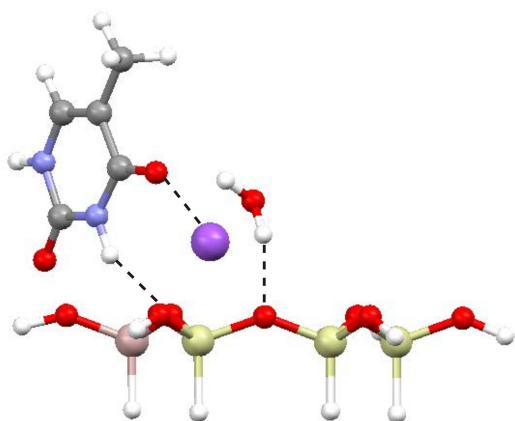
Figure 4.



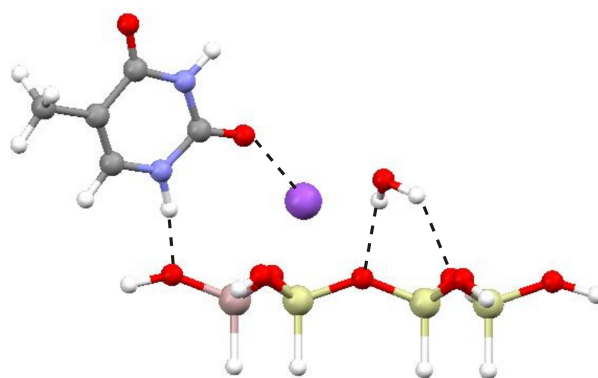
A) Na-O2(O4top)



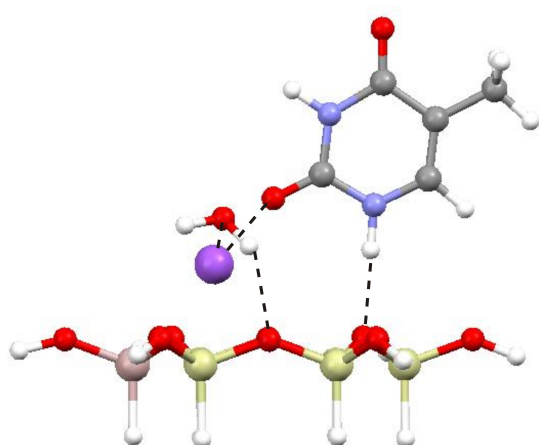
B) Na-O2



C) Na-O4



D) Na-O2(O4top)side



E) Na-O2-r

Figure 5.

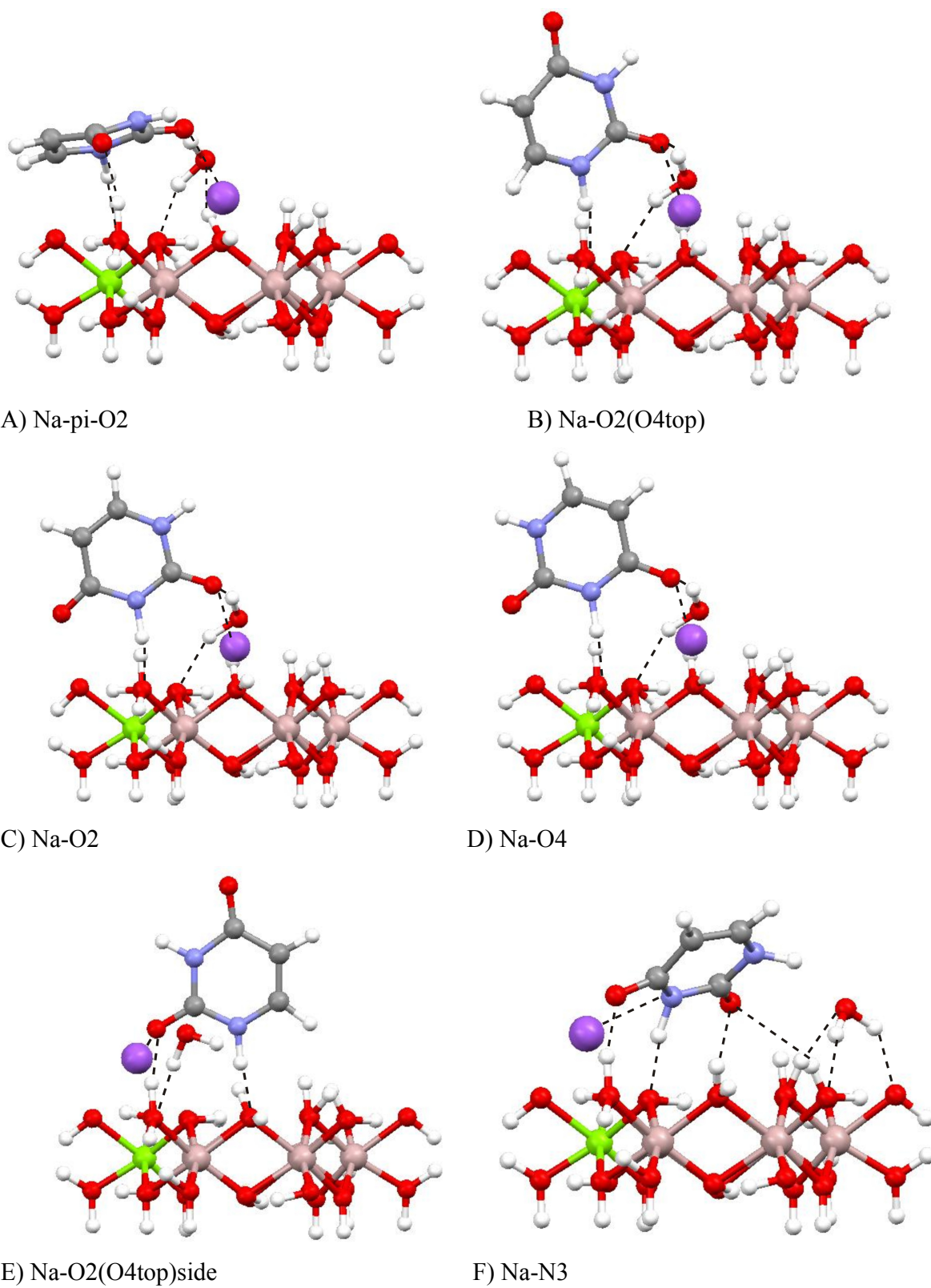


Figure 6.

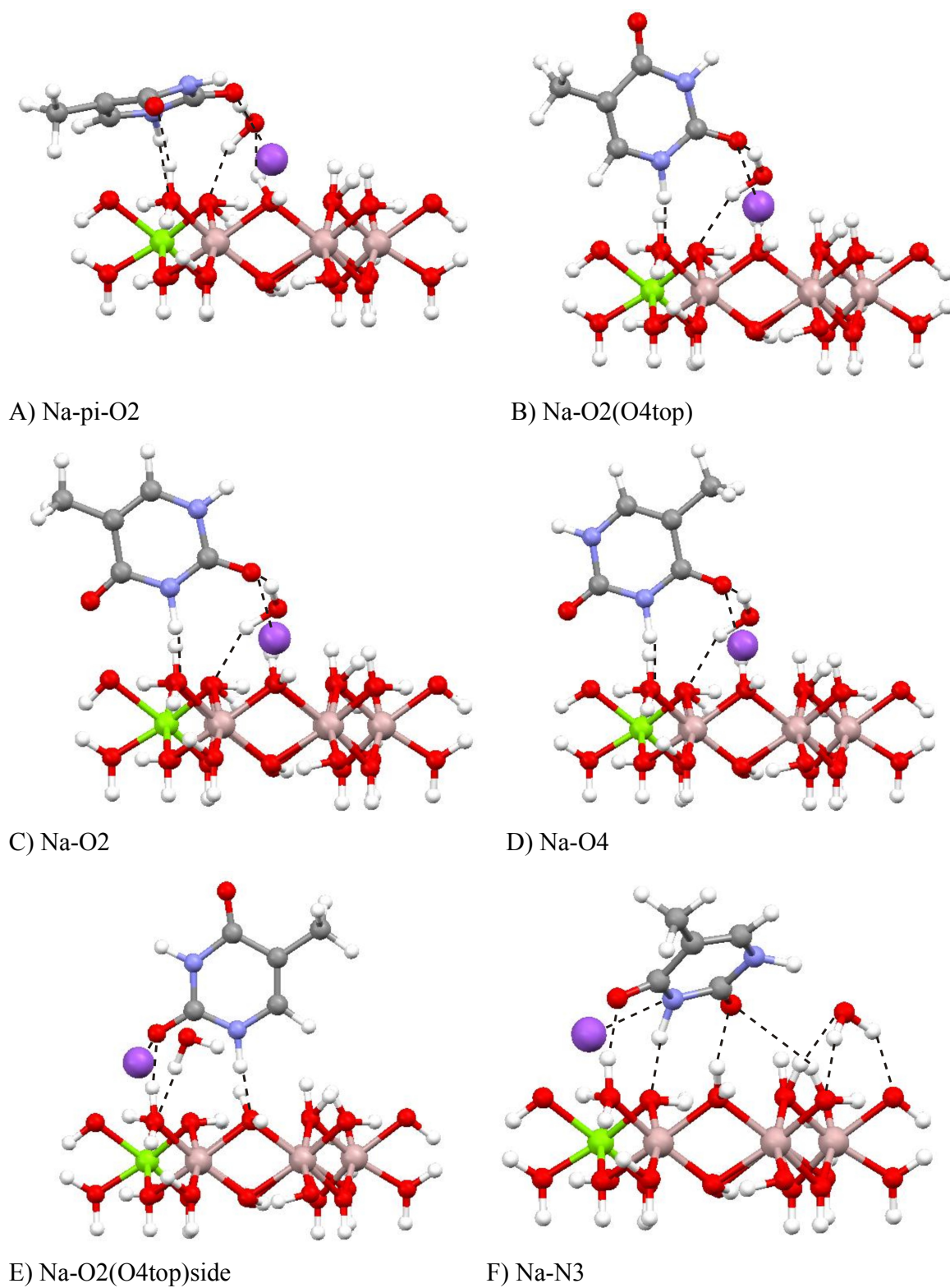


Figure 7.