Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Material

DEPOLYMERIZATION OF SODIUM POLYPHOSPHATES ON IRON OXIDE SURFACE AT HIGH TEMPERATURE

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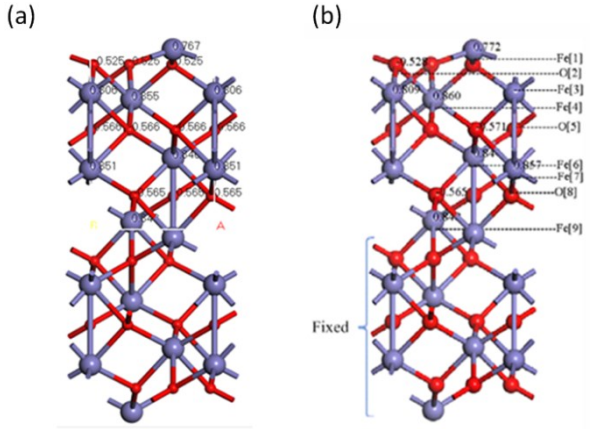

Fig. S1: Partial charges of nine top layers of Fe_2O_3 (0001) surface of (a) current work and (b) Ta *et al.*[1]

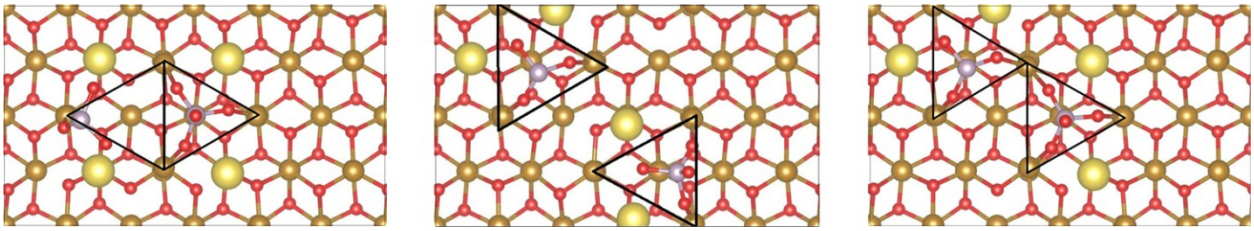

Fig. S2: Different relative position of Fe adsorption sites triangles for PO_4 or PO_3 units. The triangles can share one edge (left), be separate (middle) and share one vertex (right). Red, gold, purple and yellow spheres represent oxygen, iron, phosphorus and sodium atoms, respectively.

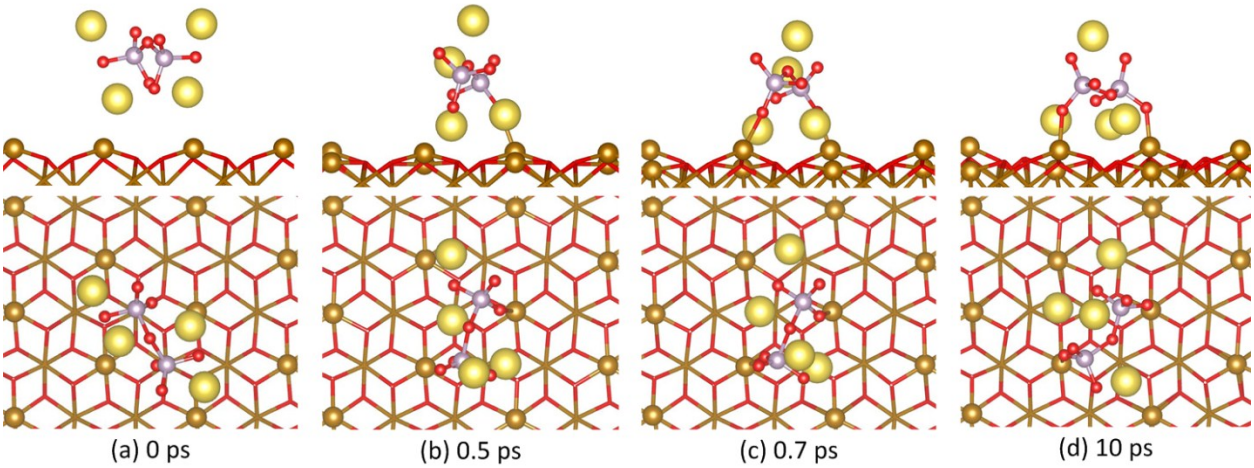

Fig. S3: Snapshots of FPMD at 300K of $Na_4P_2O_7$ cluster on Fe_2O_3 surface for 0 ps (a), 0.5 ps (b), 0.7 ps (c), and 10 ps (d). Structures have been displayed in side view (upper) and top view (lower). Red, gold, purple and yellow spheres represent oxygen, iron on top surface, phosphorus and sodium atoms, respectively. Surface oxygen and lower-layered iron atoms have been removed for apparent visualization.

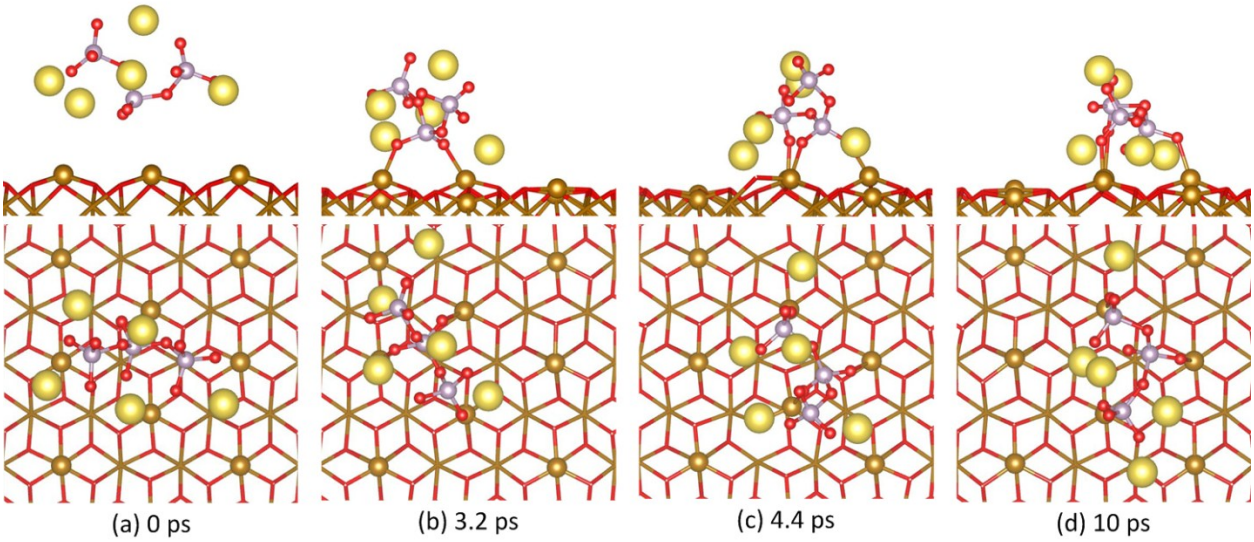

Fig. S4: Snapshots of FPMD at 300K of $Na_5P_3O_{10}$ cluster on Fe_2O_3 surface for 0 ps (a), 3.2 ps (b), 4.4 ps (c), and 10 ps (d). Structures have been displayed in side view (upper) and top view (lower). Red, gold, purple and yellow spheres represent oxygen, iron on top surface, phosphorus and sodium atoms, respectively. Surface oxygen and lower-layered iron atoms have been removed for apparent visualization.

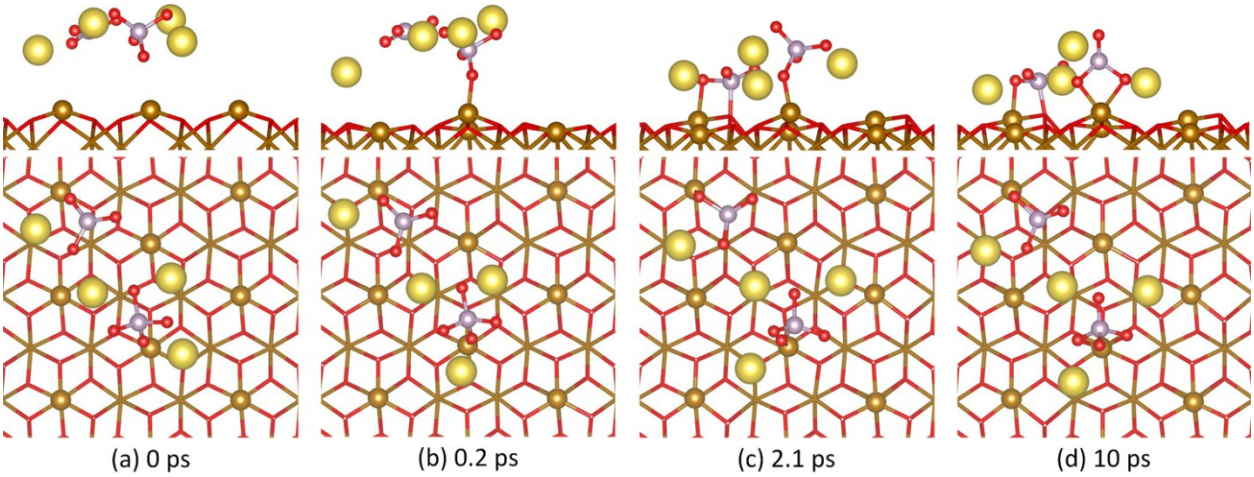

Fig. S5: Snapshots of FPMD at 300K of PO_3 and PO_4 units on Fe_2O_3 surface for 0 ps (a), 0.2 ps (b), 2.1 ps (c), and 10 ps (d). Structures have been displayed in side view (upper) and top view (lower). Red, gold, purple and yellow spheres represent oxygen, iron on top surface, phosphorus and sodium atoms, respectively. Surface oxygen and lower-layered iron atoms have been removed for apparent visualization.

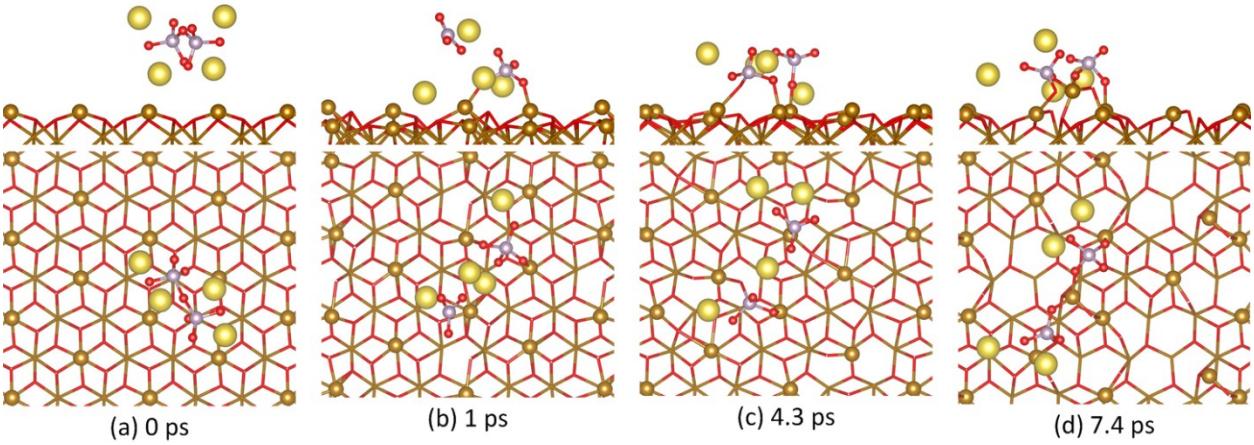

Fig. S6: Snapshots of FPMD at 1500K of $Na_4P_2O_7$ cluster on Fe_2O_3 surface for 0 ps (a), 1 ps (b), 4.3 ps (c), and 7.4 ps (d). Structures have been displayed in side view (upper) and top view (lower). Red, gold, purple and yellow spheres represent oxygen, iron on top surface, phosphorus and sodium atoms, respectively. Surface oxygen and lower-layered iron atoms have been removed for apparent visualization.

REFERENCE

1. T. D. Ta, A. K. Tieu, H. Zhu and B. Kosasih, *The Journal of Physical Chemistry C*, 2015, **119**, 12999-13010.