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

Electronic Supplemental Information for

"Adsorption of Guanidinium Collectors on Aluminosilicate Mineral–A Density Functional Study"

Naga Venkateswara Rao Nulakani[a], Prathab Baskar[b], Abhay Shankar Patra[b] and Venkatesan Subramanian[a]*

[†]Chemical Laboratory, CSIR-Central Leather Research Institute, Adyar, Chennai - 600 020, India.

[‡]Research & Development, Tata Steel Limited, Jamshedpur 831 001, India.

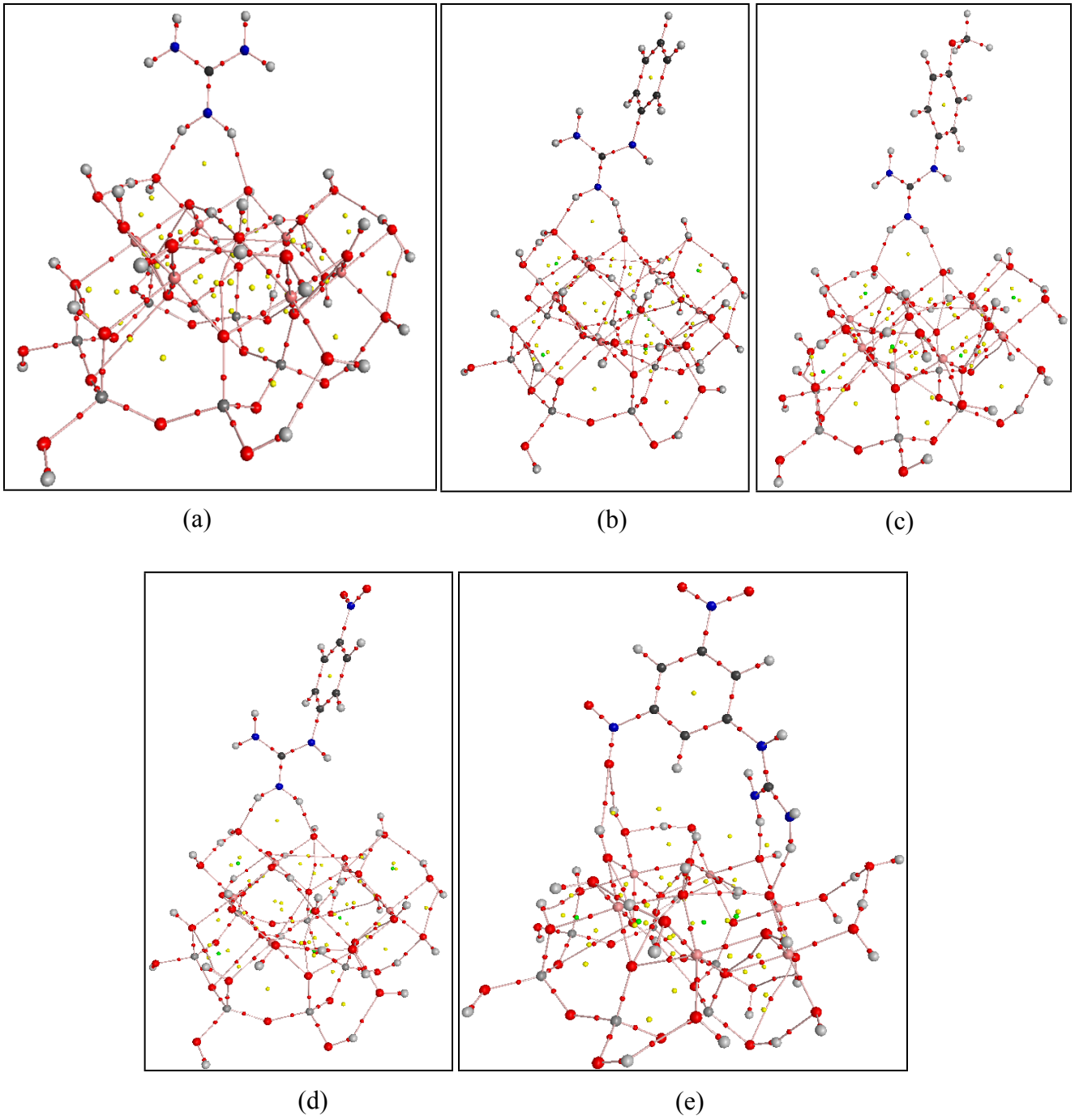


Fig. S1. The AIM analisis for various cationic collectors on K (a) surface in gas phase. (a) GC (b) PGC (c) MPGC (d) NPGC and (e) DNPGC.

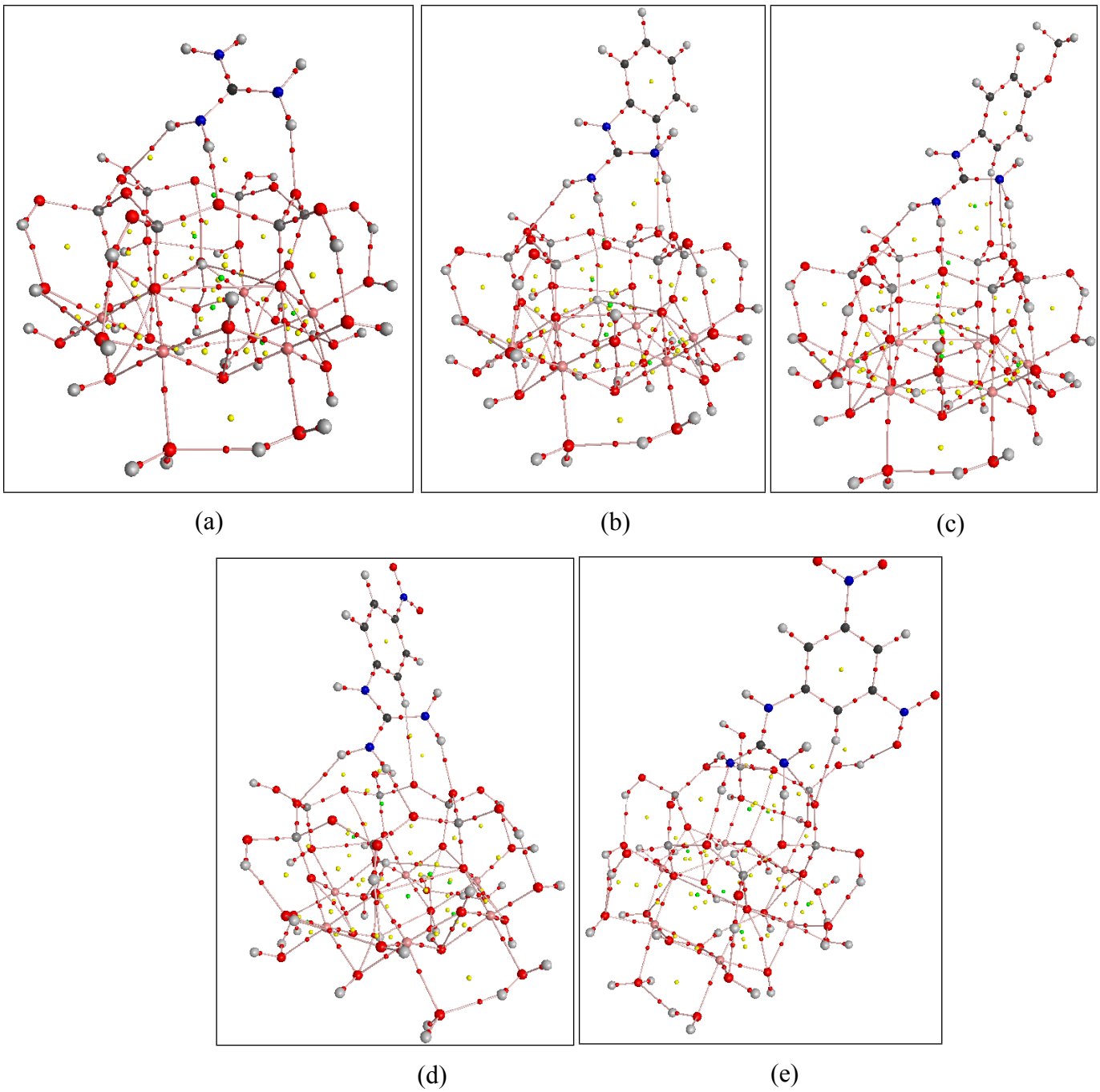
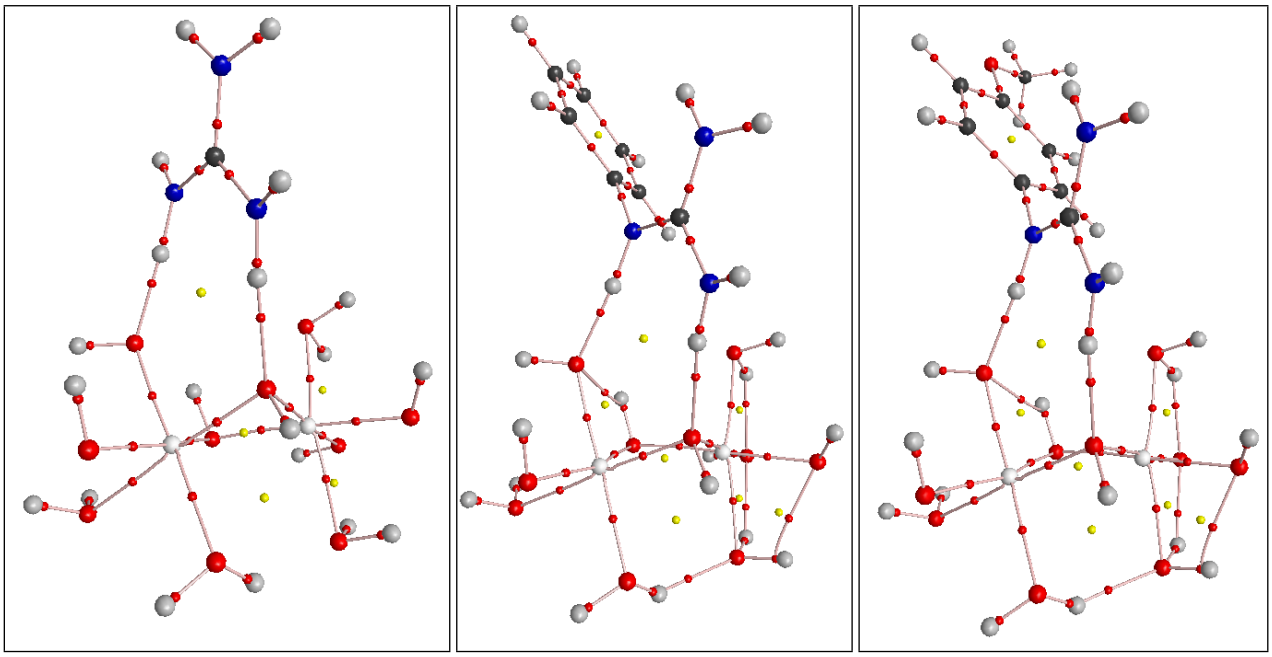
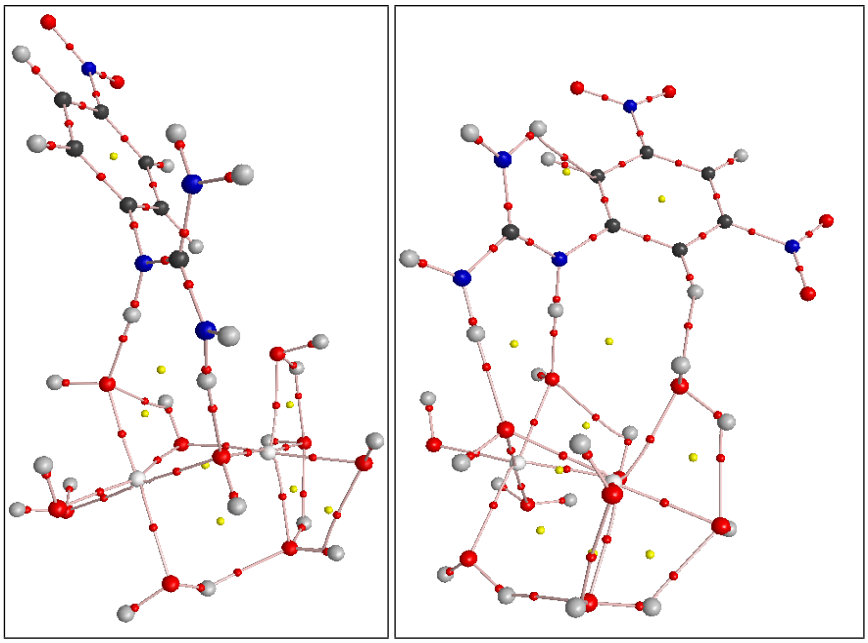


Fig. S2. The AIM plots of various cationic collectors on K (s) surface in gas phase. (a) GC (b) PGC (c) MPGC (d) NPGC and (e) DNPGC.



(a) (b) (c)



(d) (e)

Fig. S3. The AIM plots of various cationic collectors on Goethite cluster in gas phase. (a) GC (b) PGC (c) MPGC (d) NPGC and (e) DNPGC.

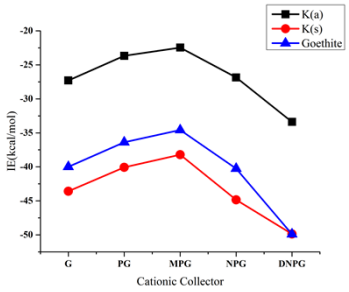
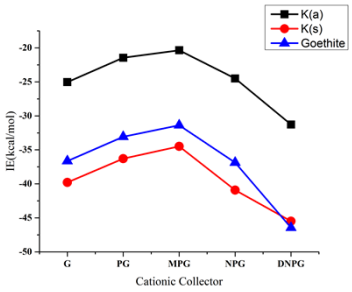
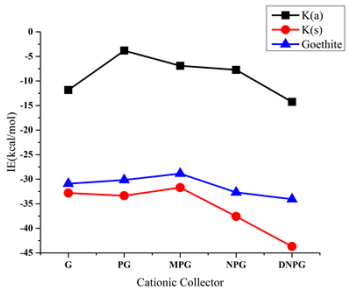
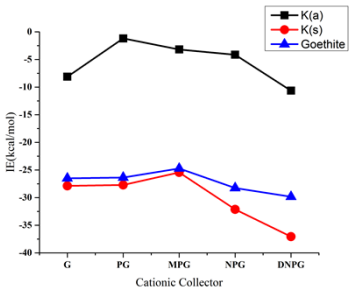
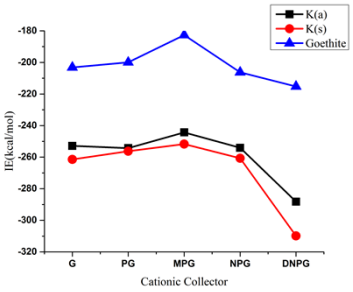
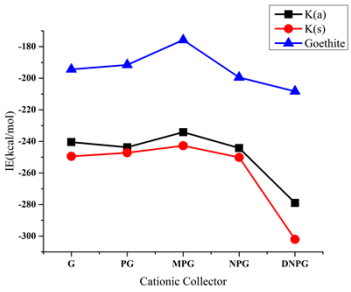
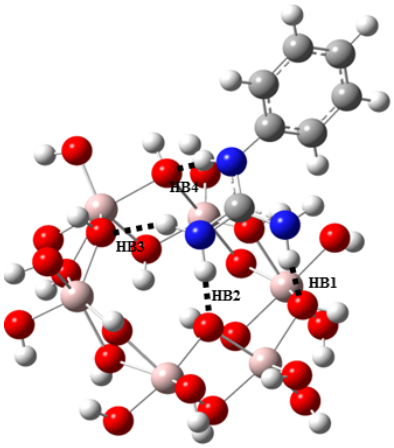
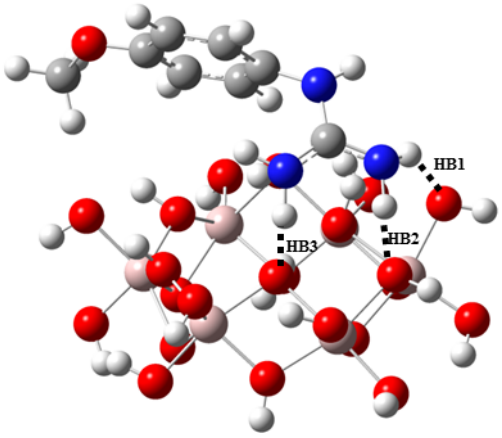
	(a) 6-31G(d,p)	(b) 6-31+G(d,p)
Gas phase		
Explicit Water model		
pH model		

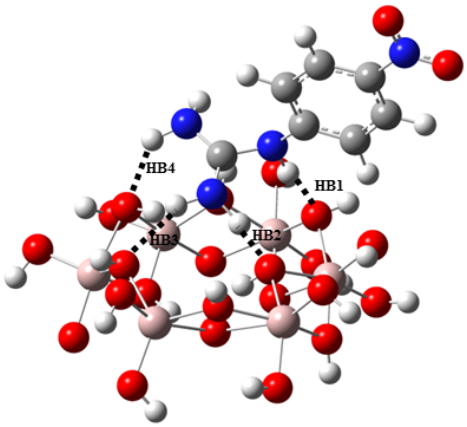
Fig. S4. The binding energy plots of five different guanidinium based cationic collectors on K(a), K(s) and goethite in gas phase, explicit water model and pH model calculated using (a) 6-31G(d,p) and (b) 6-31G+(d,p) basis sets.



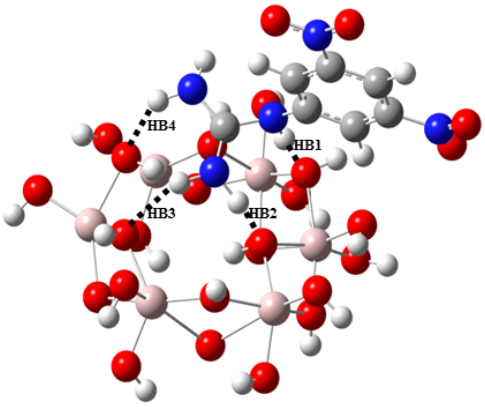
(a) PGC on K (a)



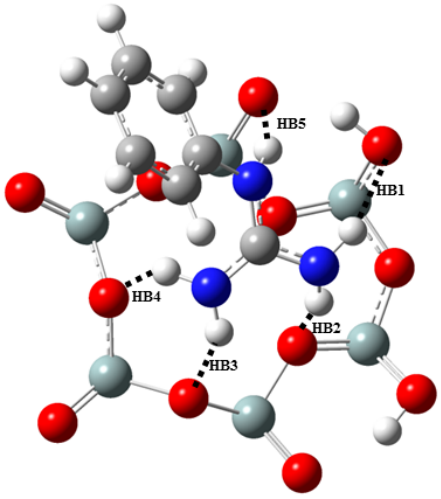
(b) MPGC on K (a)



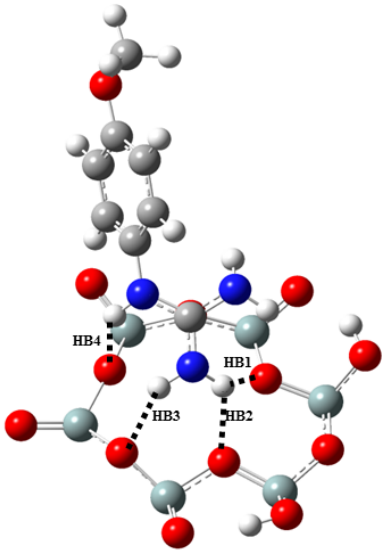
(c) NPGC on K (a)



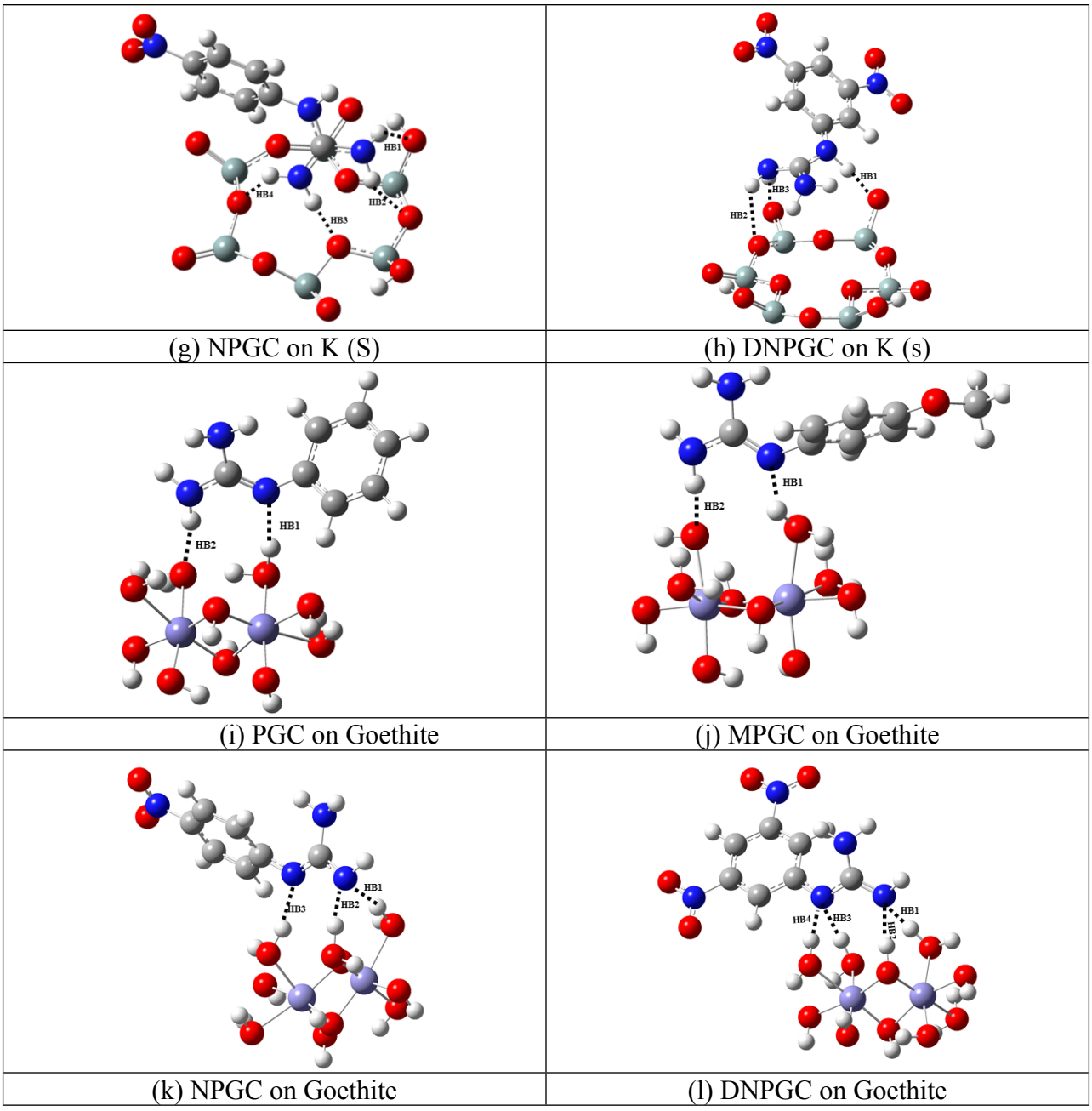
(d) DNPGC on K (a)



(e) PGC on K (S)



(f) MPGC on K (S)



(g) NPGC on K (S) | (h) DNPGC on K (s)

(i) PGC on Goethite | (j) MPGC on Goethite

(k) NPGC on Goethite | (l) DNPGC on Goethite

Fig. S5. The optimized geometries of four cationic coleectors (PGC, MPGC, NPGC and DNPGC) on three inorganic mineral surfaces in pH mode.