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

Supplementary Information

Adsorption and exchange reactions of iodine molecules at the alumina surface: modelling alumina-iodine reaction mechanisms

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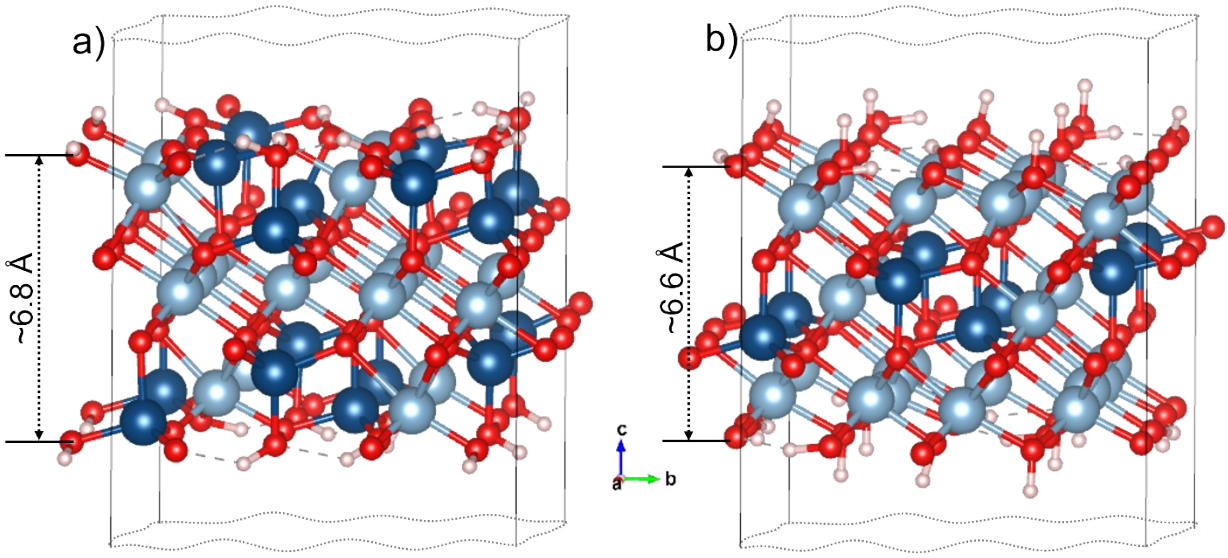

Figure S1. Structures of periodic slab models of two γ-Al_2O_3 representing two surfaces parallel to (111) plane used in the DFT calculations. a) Slab_A, terminated with surface plane A (sites Ia, IIa), and b) Slab_B, terminated with surface plane B (sites Ib, IIb, and III). Notification of surfaces and sites according to H. Knözinger and P. Ratnasamy, *Catal. Rev.*, 1978, **17**, 31–70. Vertical shadow lines represent computational cell boundaries (details are given in Table S1). Color scheme: red – oxygen atoms, white – hydrogen atoms, blue – Al_{VI} atoms, and dark blue – Al_{IV} atoms.

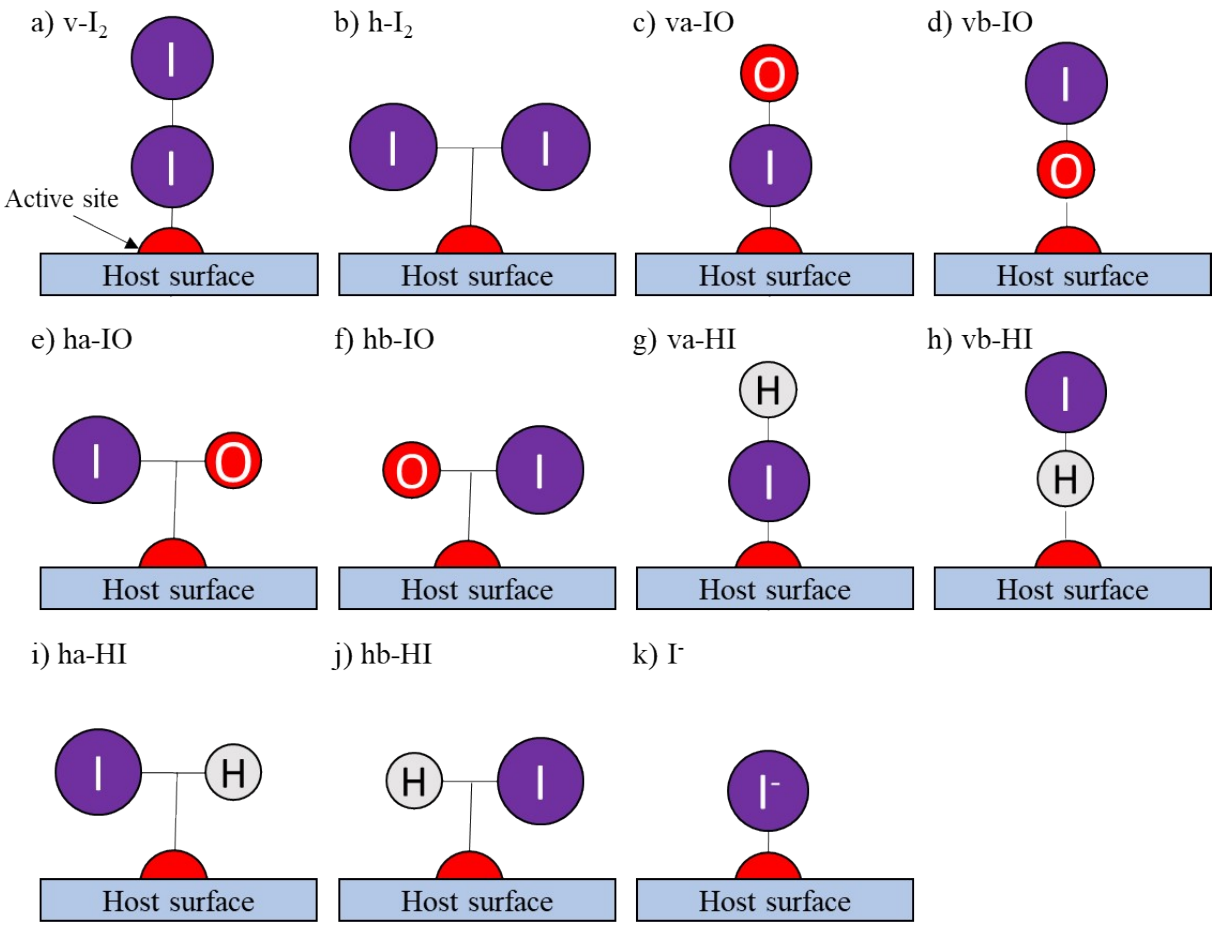

Figure S2. Schematic representation of initial positions and geometries of vertical (v) and horizontal (h) arrangements of each molecule relative to the alumina host surface. Spheres represent atoms labeled accordingly (I=iodine, H=hydrogen, and O=oxygen). Red sphere at the host surface is an oxygen atom from active OH site. a) v-I_2, b) h-I_2, c) va-IO, d) vb-IO, e) ha-IO, f) hb-IO, g) va-HI, h) vb-HI, i) ha-HI, j) hb-HI and k) I^-.

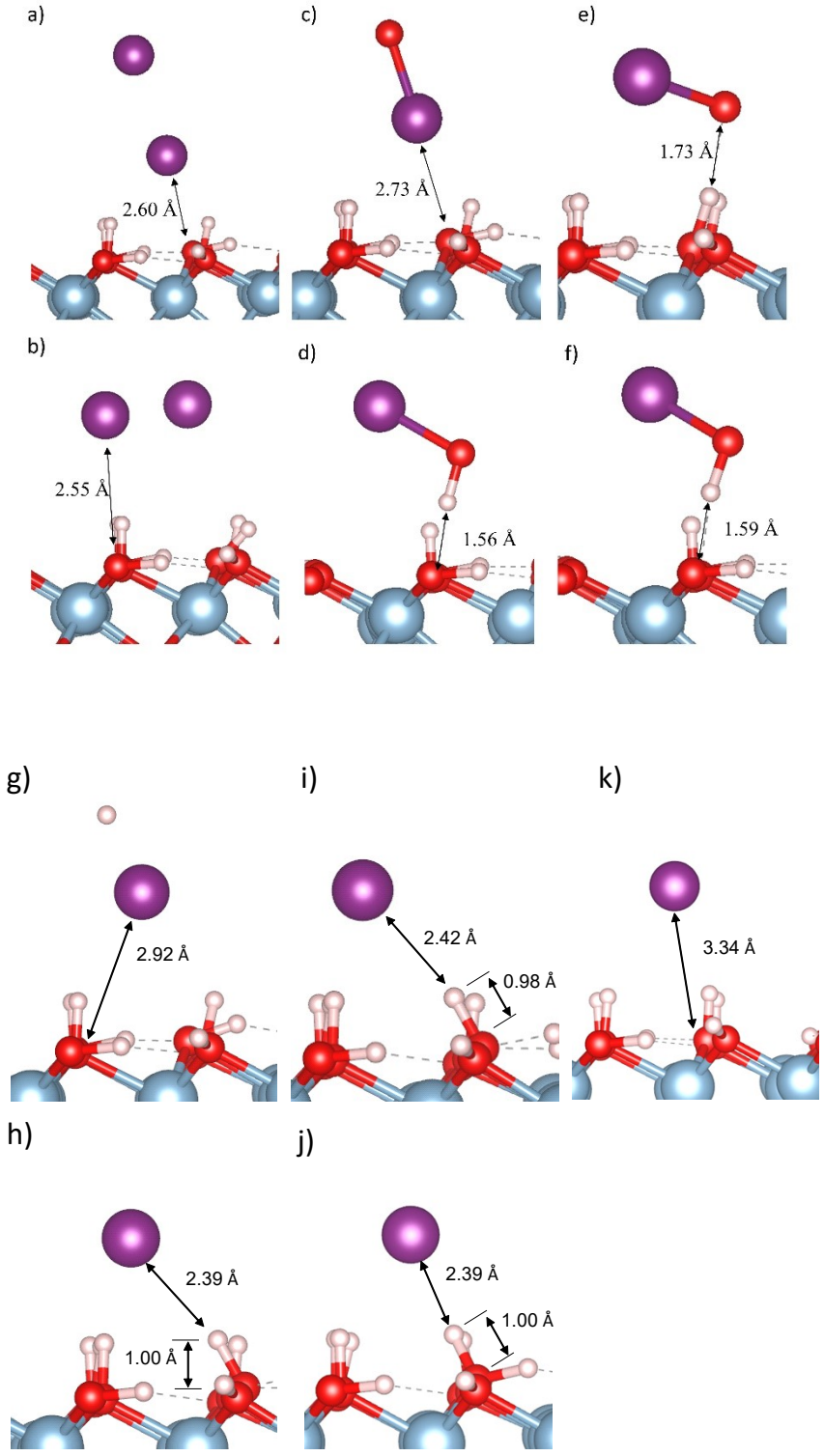

Figure S3. Optimized structures of iodine species at the Ib site.

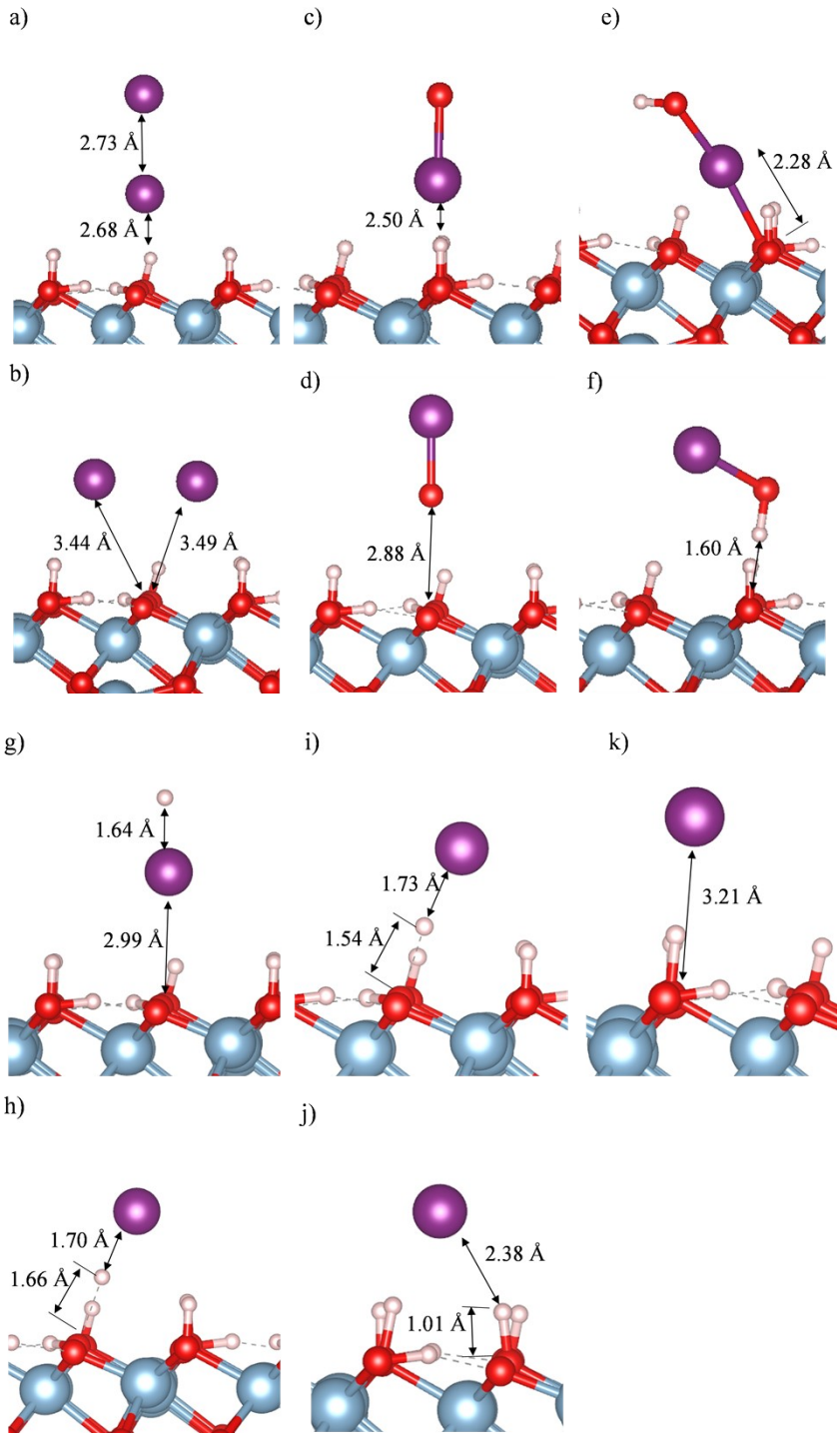

Figure S4. Optimized structures of iodine species at the IIb site.

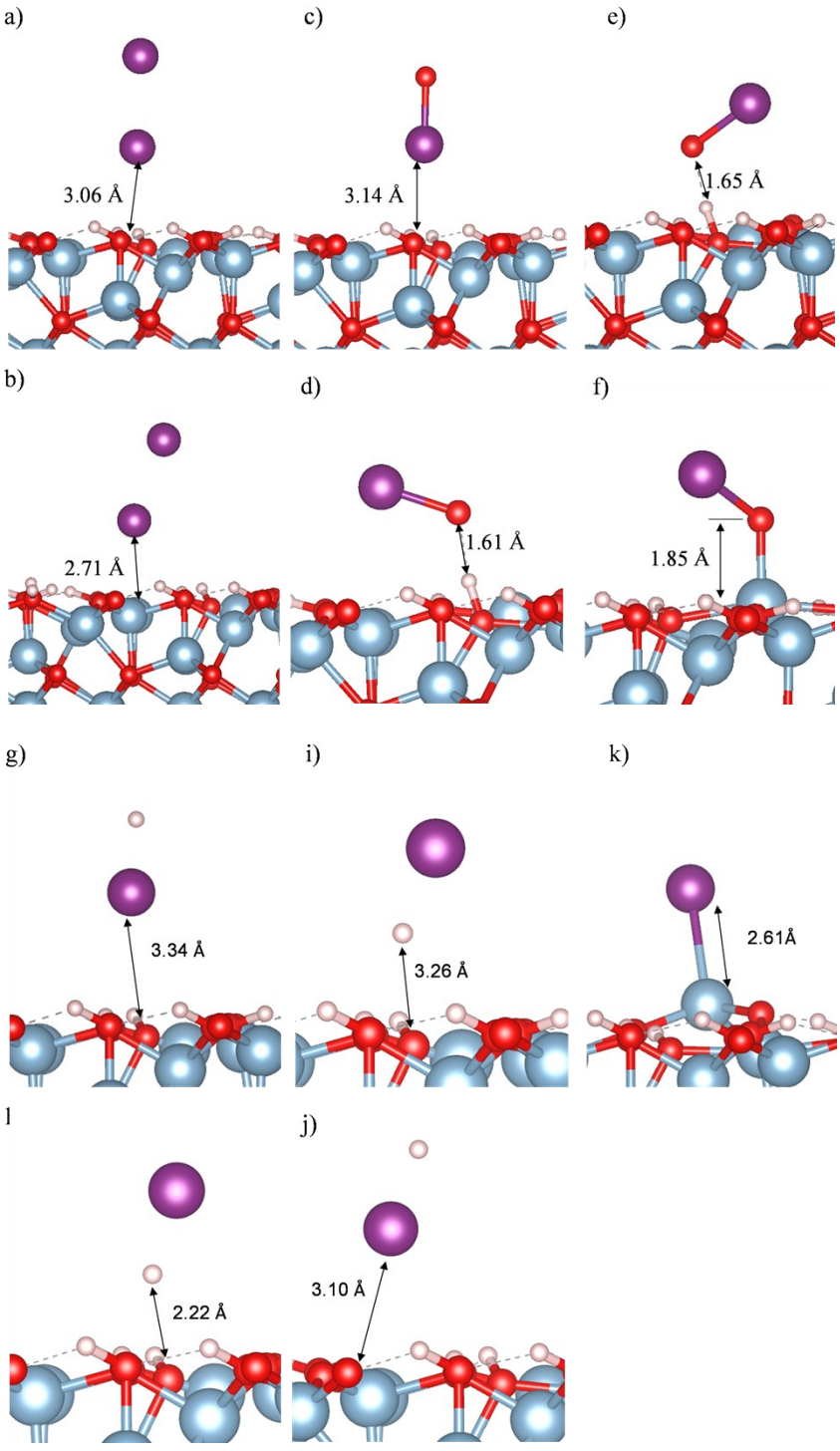

Figure S5. Optimized structures of iodine species at the Ia site.

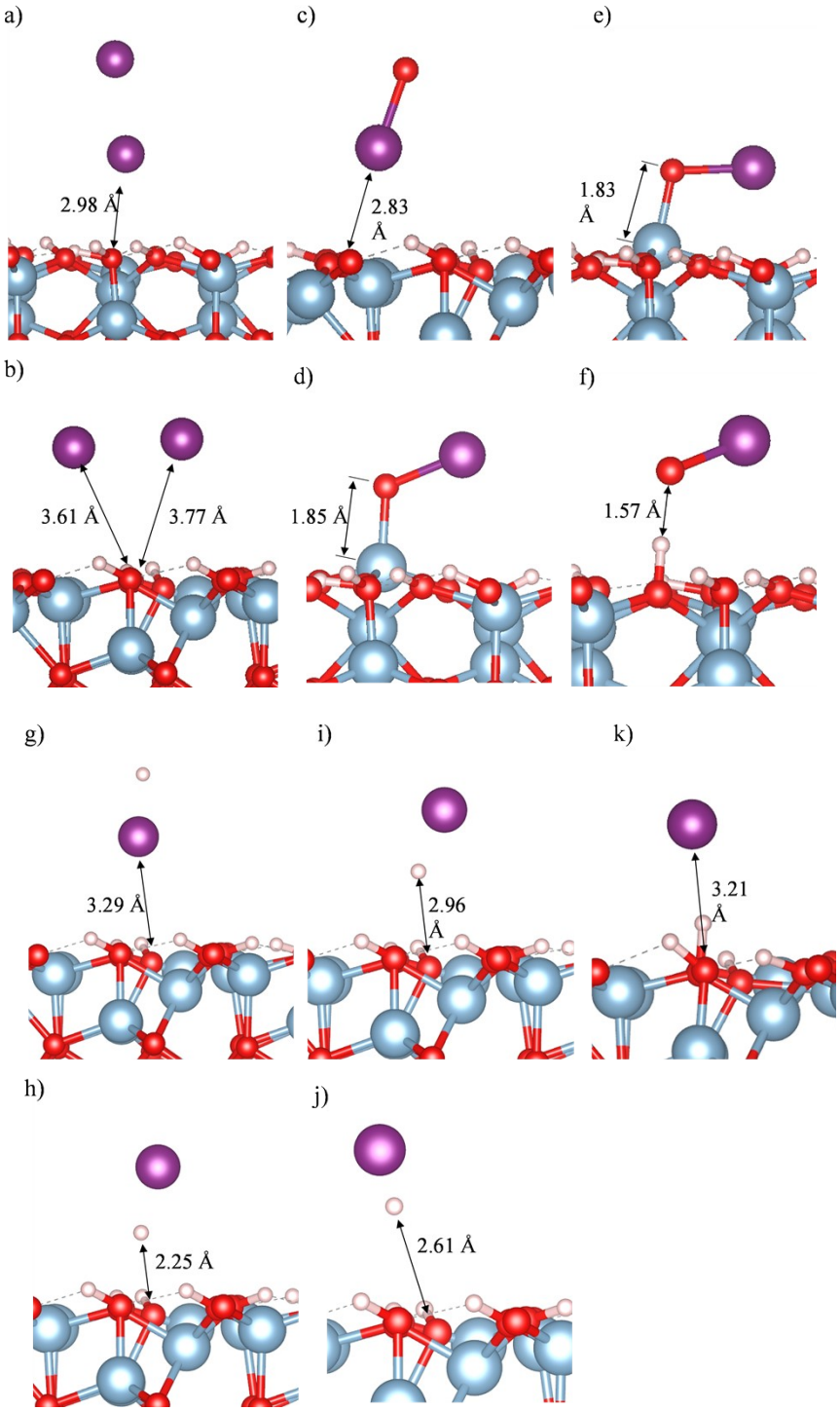

Figure S6. Optimized structures of iodine species at the IIa site.

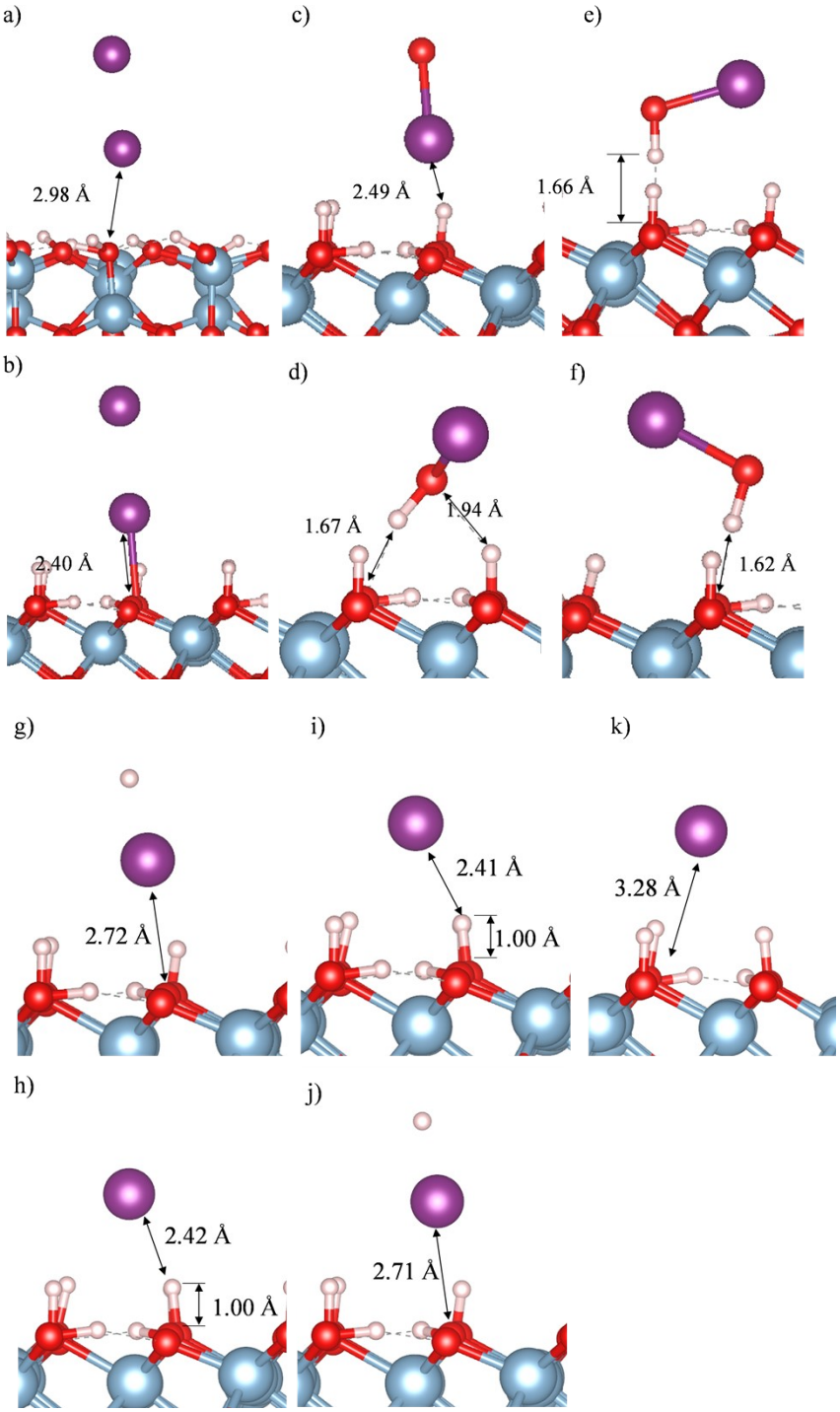

Figure S7. Optimized structures of iodine species at the III site.

Table S1. Details of rectangular computational cells of two periodic slab models used in the DFT calculations (See also Fig. S1).

	Slab_A	**Slab_B**
Sites	Ia and IIa	Ib, IIb and III
a (Å)	11.23	
b (Å)	9.72	
c (Å)	40.00	
Number of atoms	120	