Supporting information

For

Recycling of zincite (ZnO) via uptake of hydrogen halides

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Figure S1. Relative energy profile diagram for the first addition step of HCl (Blue) and HBr (Red) molecules over ZnO (1010) surface using the energy cut-off of 400 eV. Values in brackets are for cut-off of 320 eV.



Figure S2. Relative energy profile diagram for the first addition step of HCl (Blue) and HBr (Red) molecules over ZnO ($10\overline{1}0$) surface using a (3×3) unit cell. Values in brackets are for (2×2) unit cell.



Figure S3. Slab models of ZnO(1010) and (0001) surfaces. (a) ZnO unit cell; (b) side and top view ZnO(1010); (c) side and top view ZnO (0001). The green and red spheres represent zinc and oxygen atoms, respectively.



Figure S4. Optimized structures of gaseous ZnCl₂ (left) and ZnBr₂ (right) molecules.



Figure S5. Arrhenius plots for reactions of zincite $(10\overline{1}0)$ surface with HCl molecules (a) and HBr molecules (b).



Figure S6. (a) TG-DTG curve of ZnO-PVC mixture, (b) Effect of temperature on effectiveness of zinc bromination released from TBBPA during thermal treatment of ZnO:TBBPA ^{37, 77}.