Supporting information

How do organic gold compounds and organic halogen molecules interact? Comparison with hydrogen bonds

MengGao, Qingzhong Li*, Hai-Bei Li*, Wenzuo Li, Jianbo Cheng

Figure list

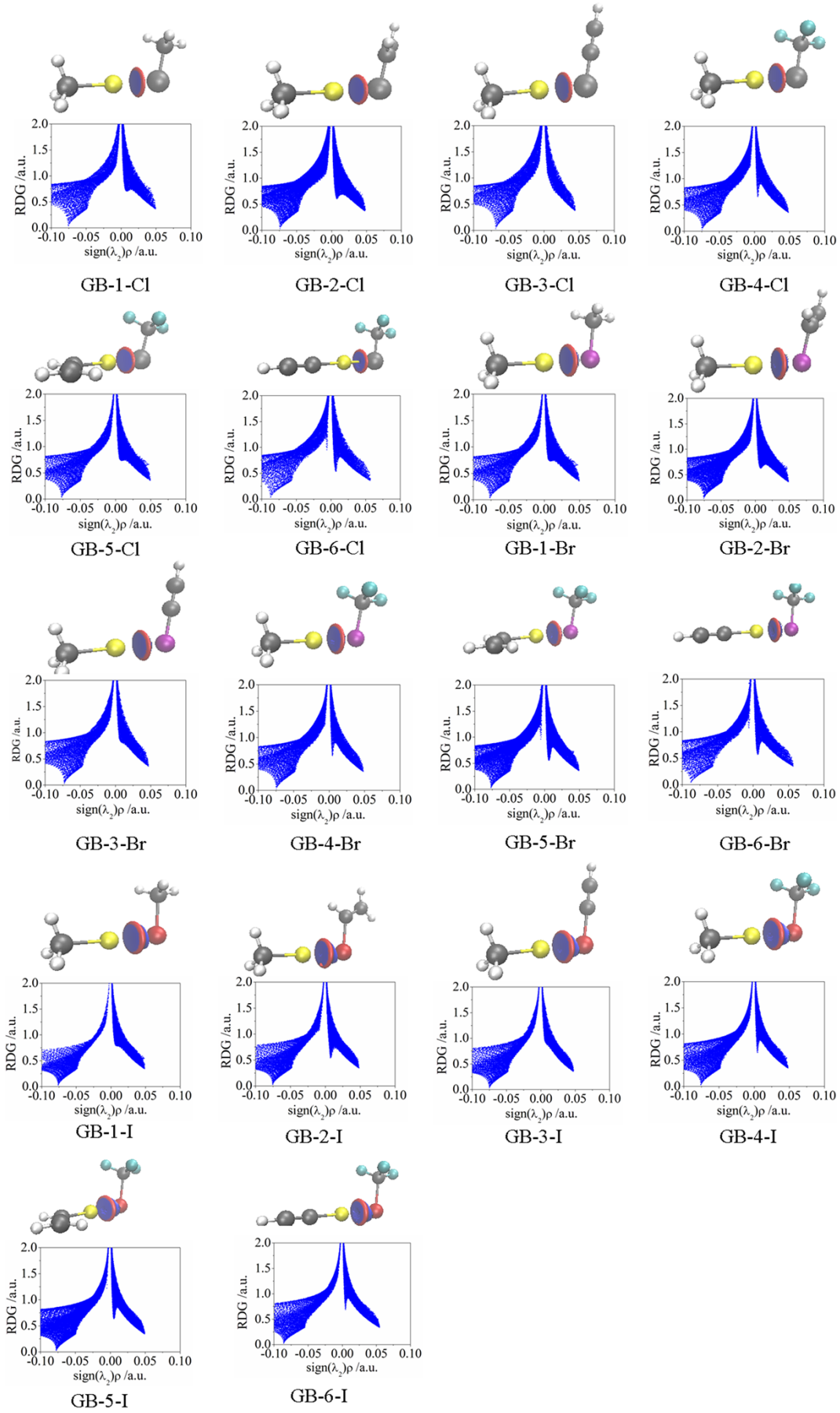

Fig. S1. Gradient isosurfaces (s =0.1 au) and plots of the reduced density gradient (RDG) versus the electron density multiplied by the sign of the second Hessian eigenvalue in GBs.

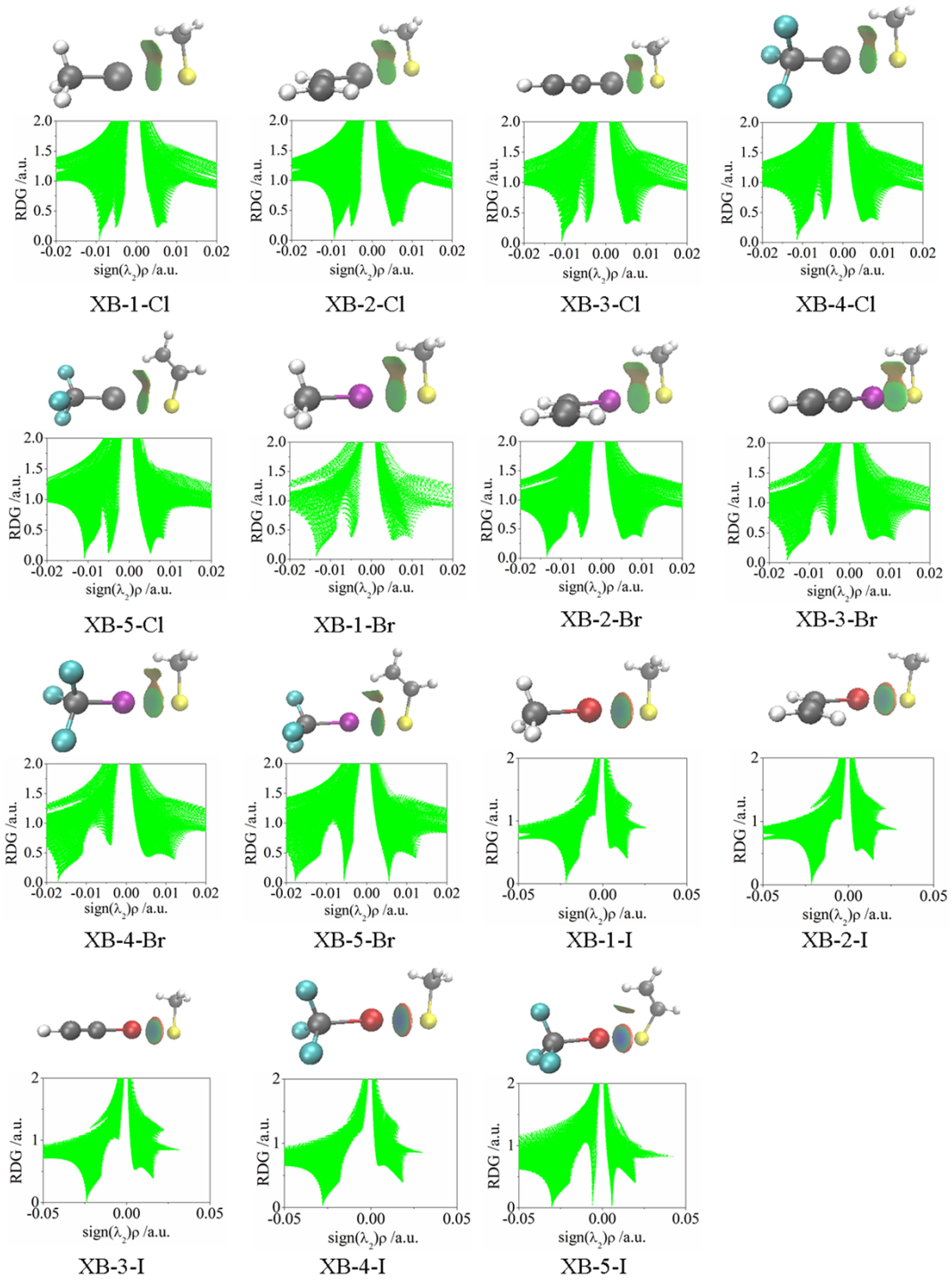

Fig. S2. Gradient isosurfaces (s =0.1 au) and plots of the reduced density gradient (RDG) versus the electron density multiplied by the sign of the second Hessian eigenvalue in XB-1-Br.

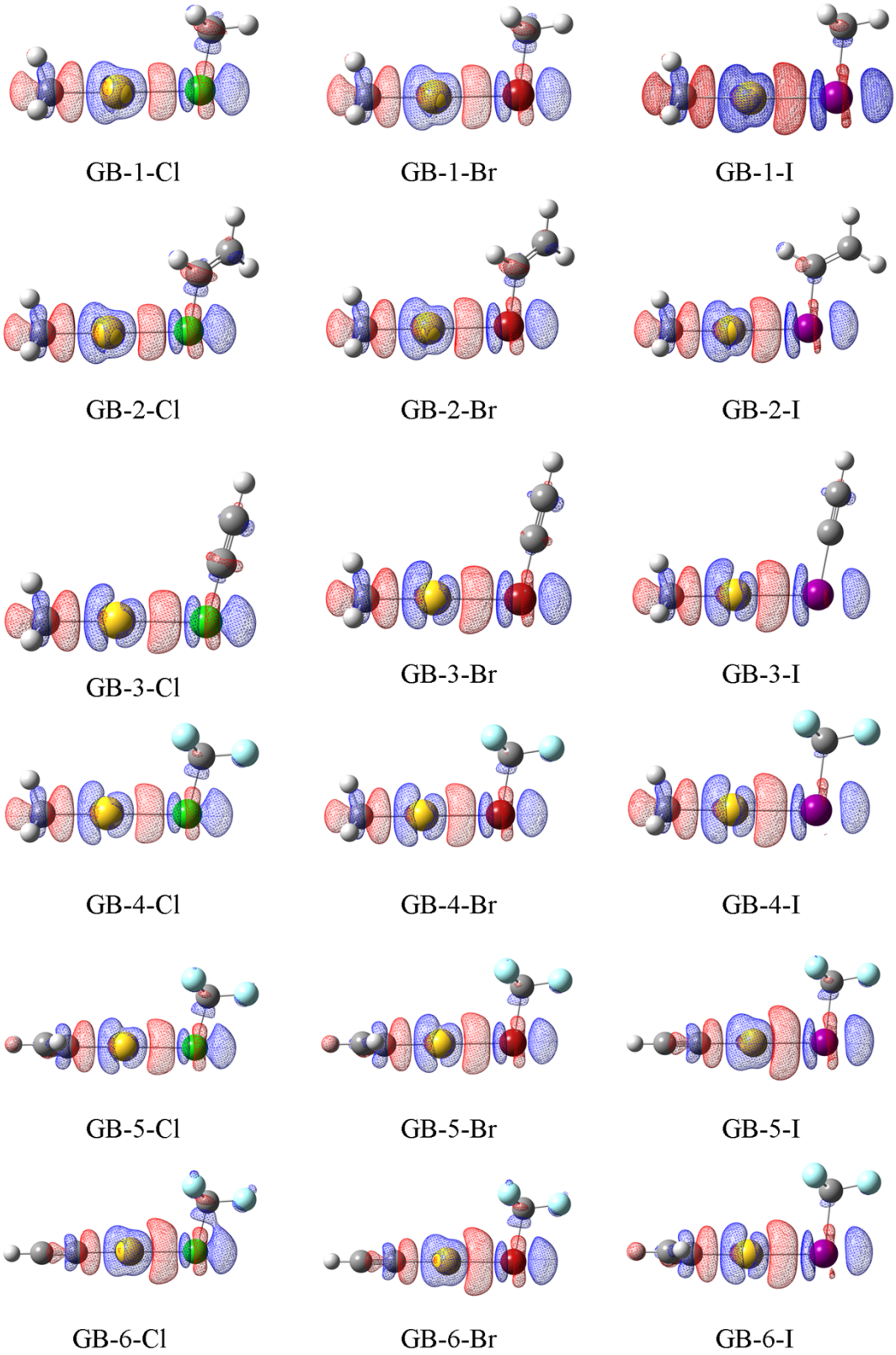

Fig. S3. Electron density differences of GBs (iso=0.002) in all systems. Red regions indicate increased electron density, while blue regions represent decreased electron density.

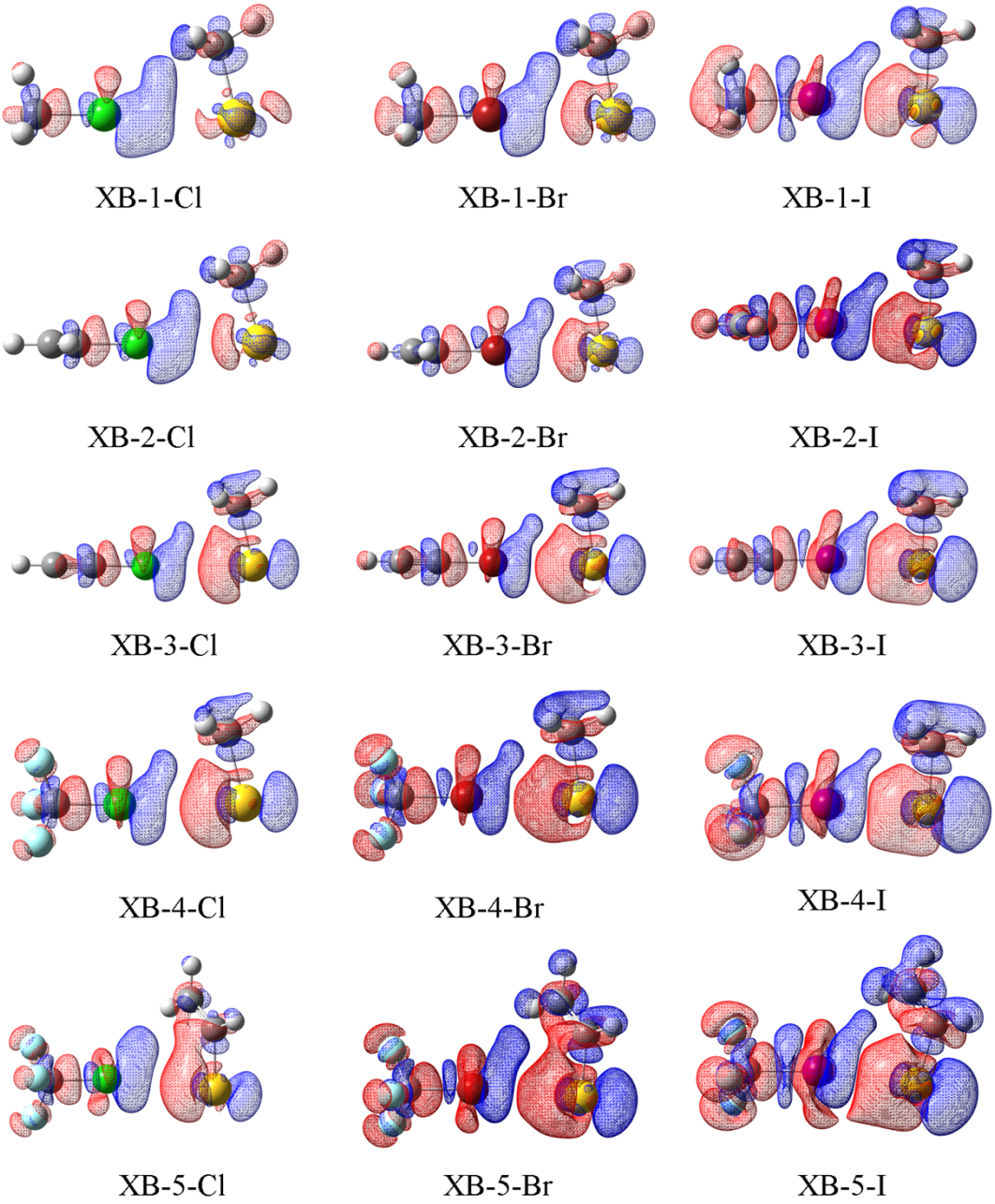

Fig. S4. Electron density differences of XBs (iso=0.0002) in all systems. Red regions indicate increased electron density, while blue regions represent decreased electron density.