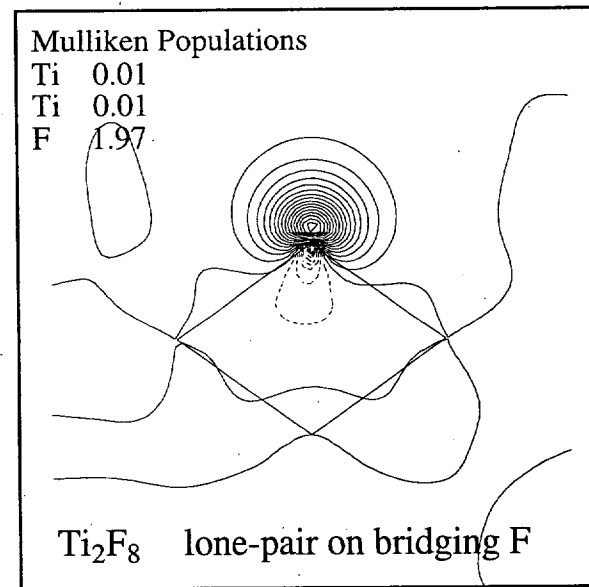
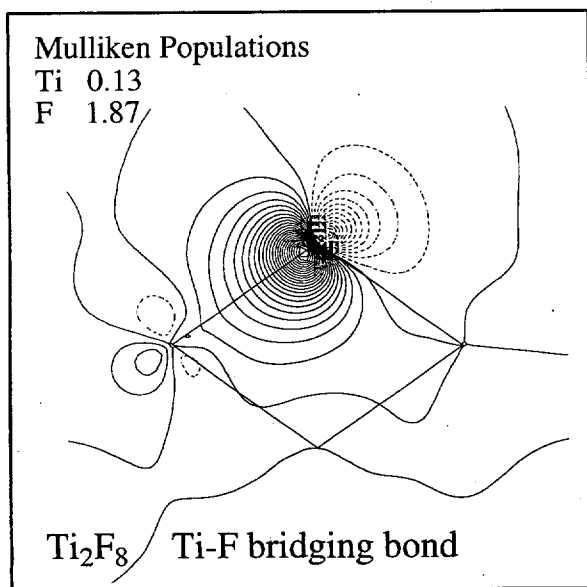
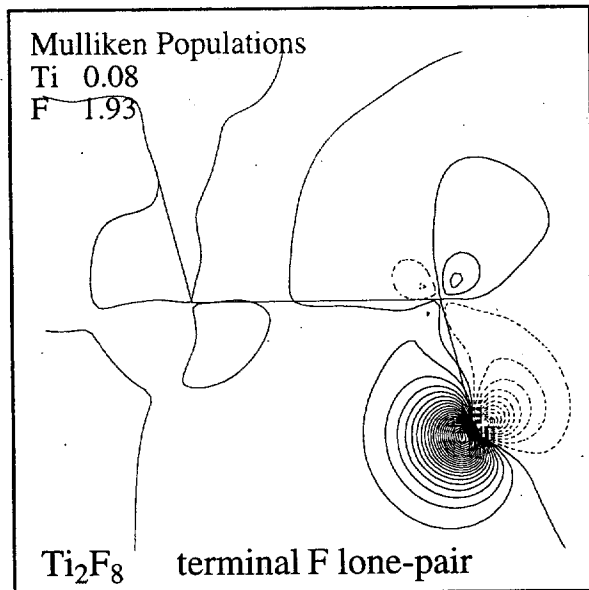
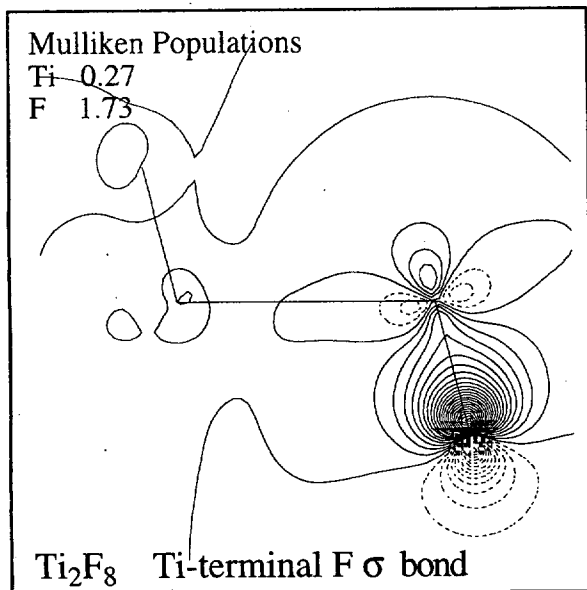
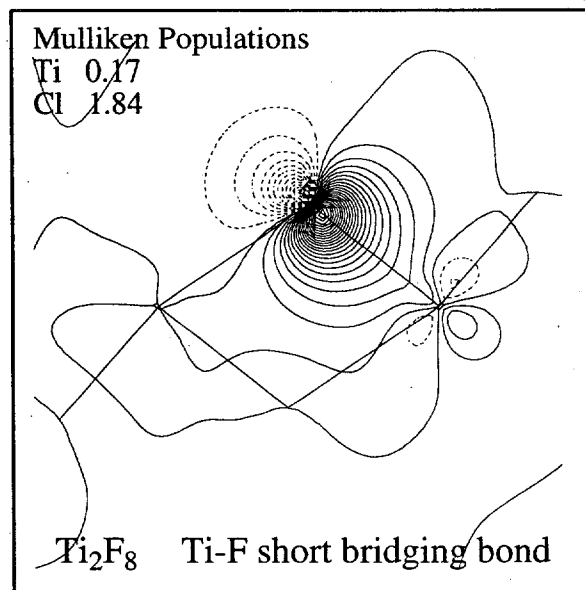
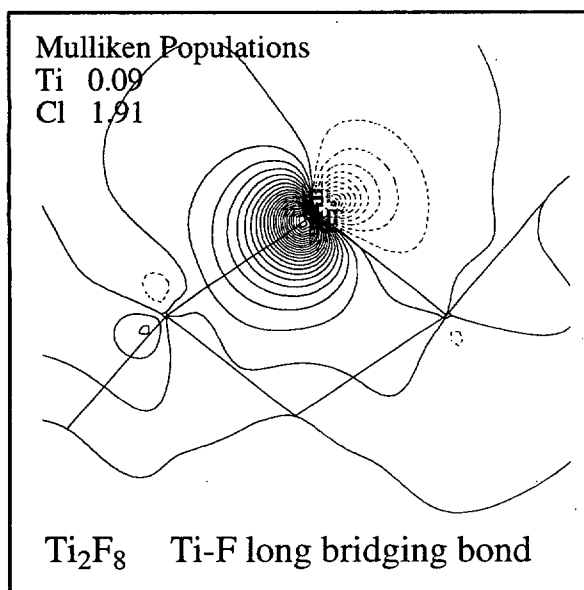


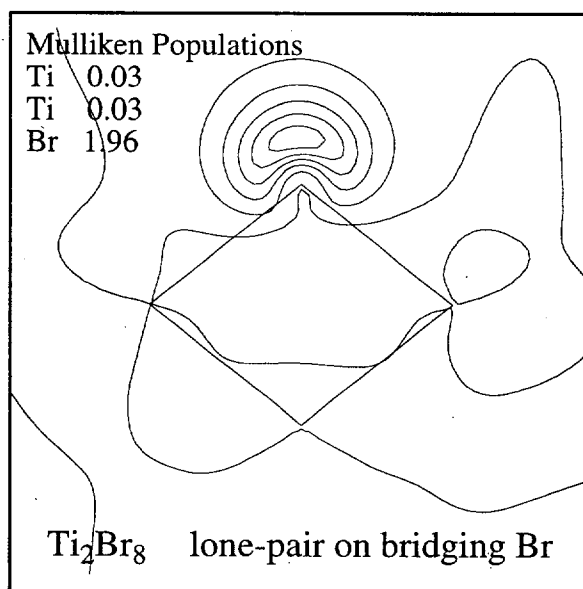
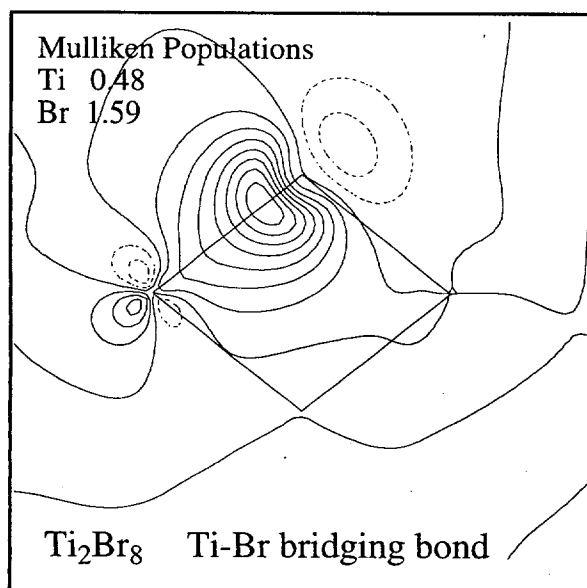
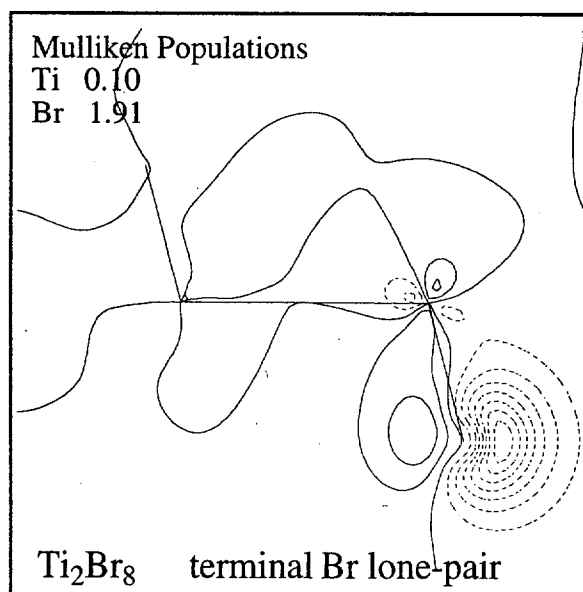
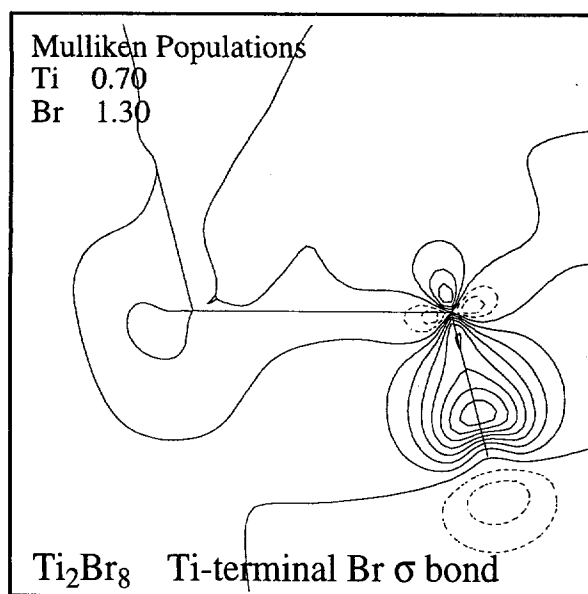
S1. LMO plots of Ti-X σ -bonds and X lone-pairs in TiX₄ (X=F,Br).
The contour increments are 0.05 Bohr^{3/2}.



S2. LMO plots of a Ti-F σ -bond, F lone-pairs, and a Ti-F bridging bond in the Ti₂F₈ transition state. The contour increments are 0.05 Bohr^{3/2}.



S3. LMO plots of short and long Ti-F bridging bonds in the Ti₂F₈ minimum. The contour increments are 0.05 Bohr^{3/2}.



S4. LMO plots of a Ti-Br σ -bond, Br lone-pairs, and a Ti-Br bridging bond in the Ti₂Br₈ transition state. The contour increments are 0.05 Bohr^{3/2}.