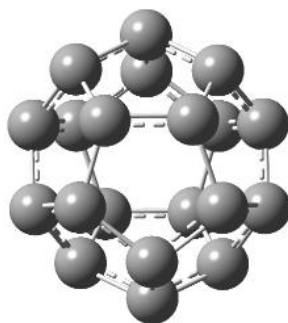
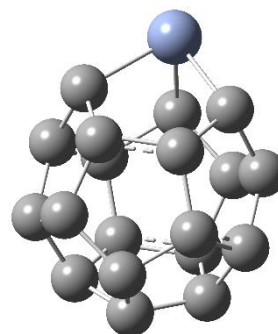


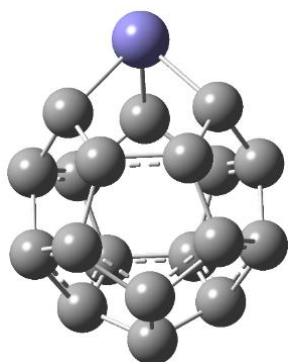
WAR



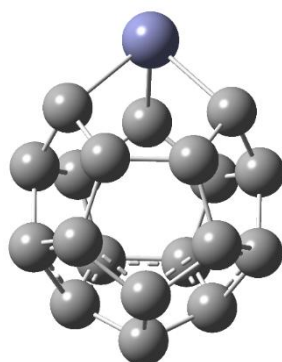
C20



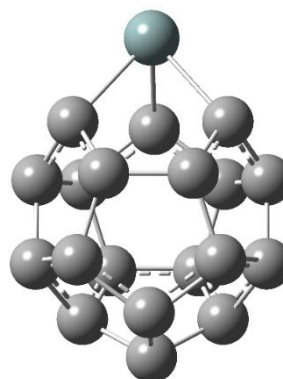
CrC19



FeC19



NiC19



SiC19

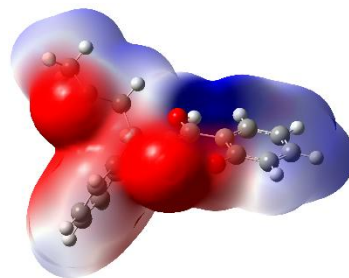
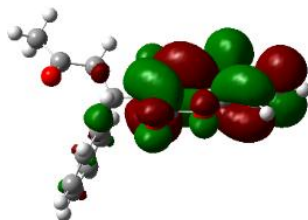
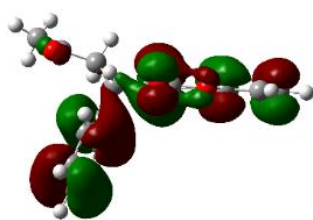
Fig. S1. Optimized geometry of WAR, C20, and MC19.

HOMO

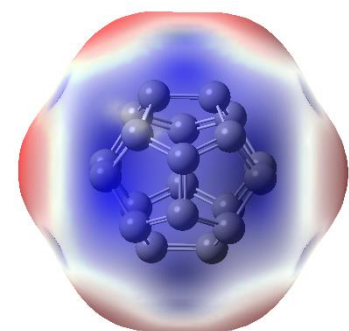
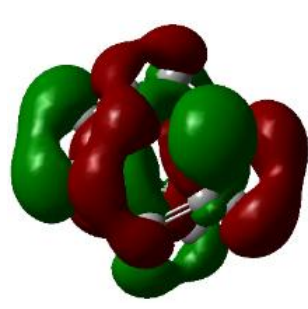
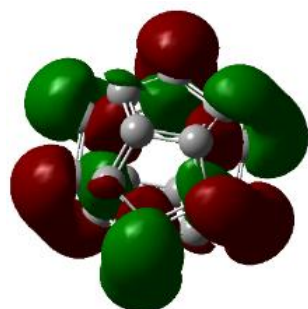
LUMO

MEP

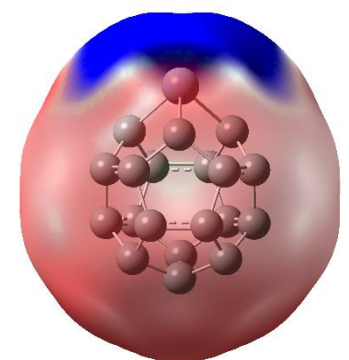
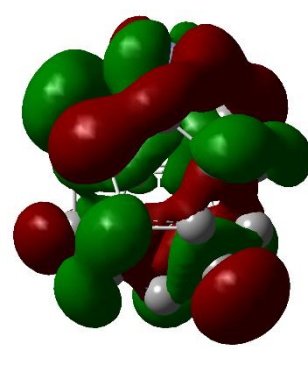
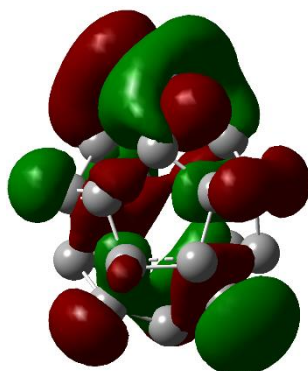
WAR



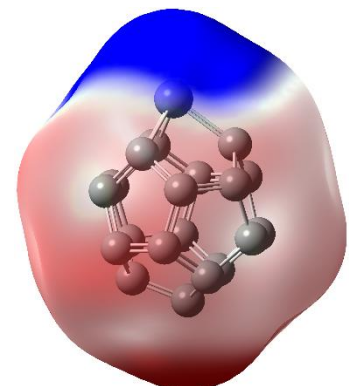
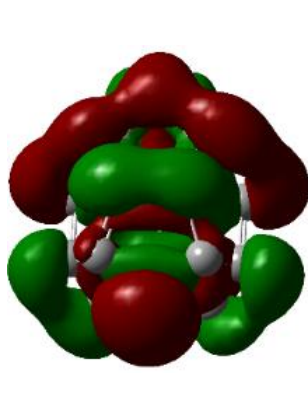
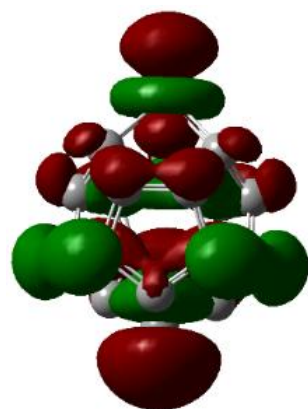
C20



CrC19



FeC19



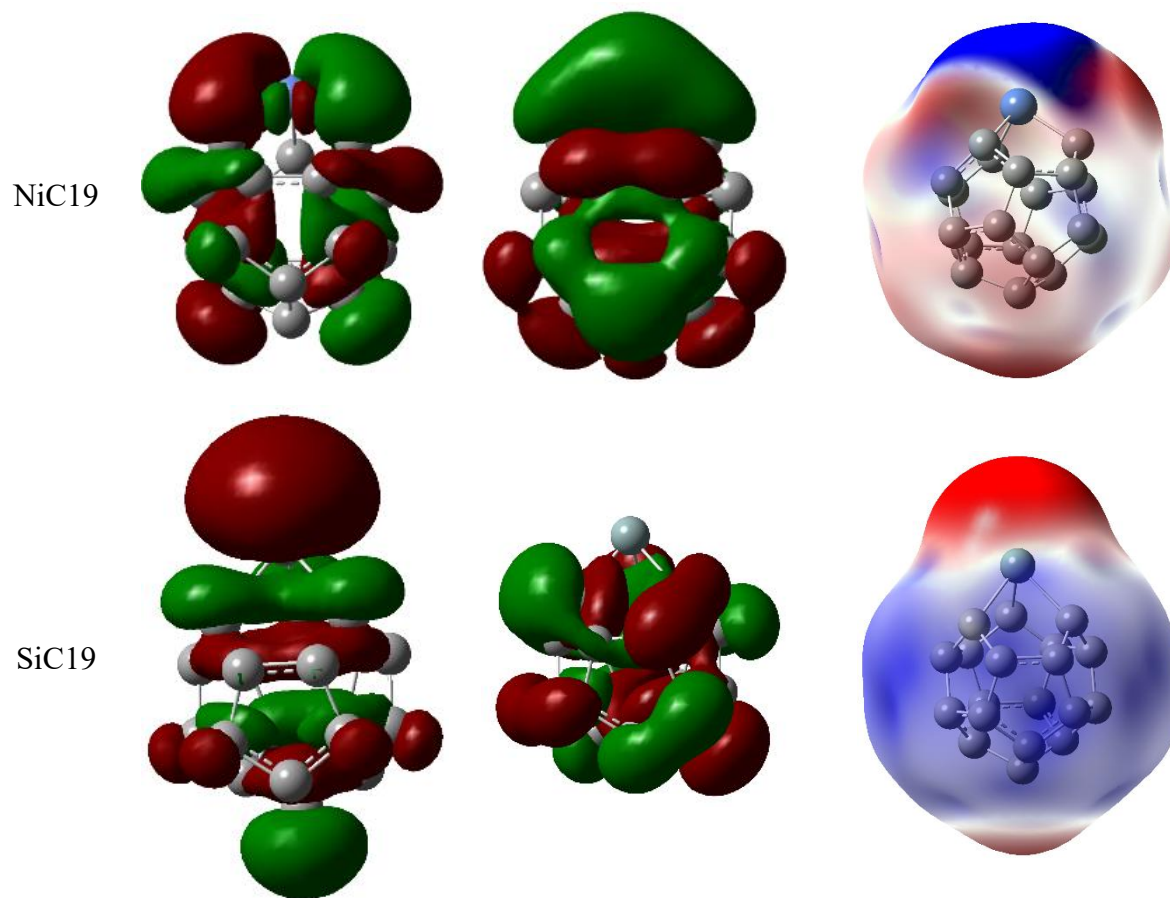
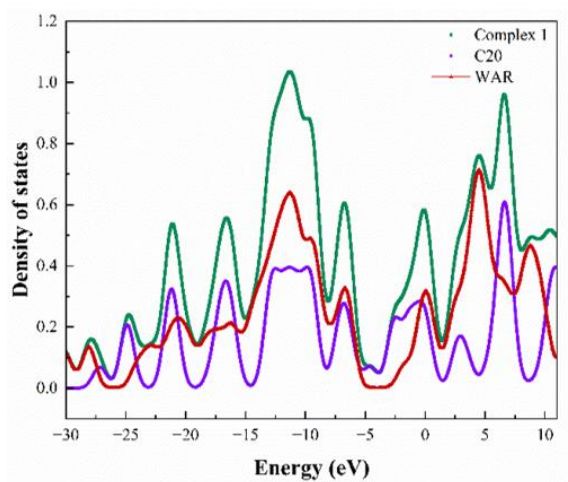
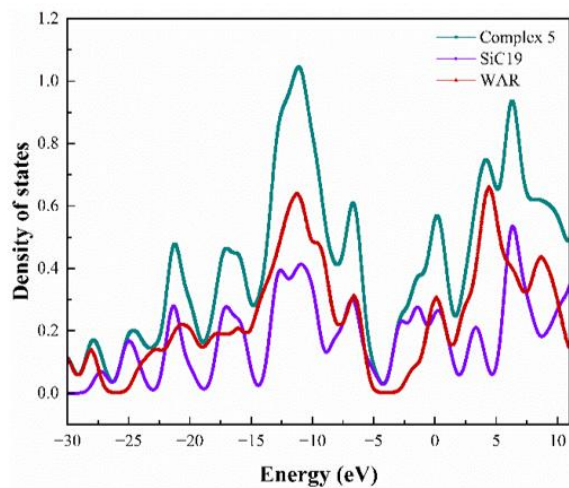


Fig. S2. Diagram of HOMO and LUMO orbitals and Molecular electrostatic potential maps for WAR, C20, and MC19.



Complex 1



Complex 5

Fig. S3. Calculated electron density states TDOS and PDOS for Complex 1 and Complex 5.

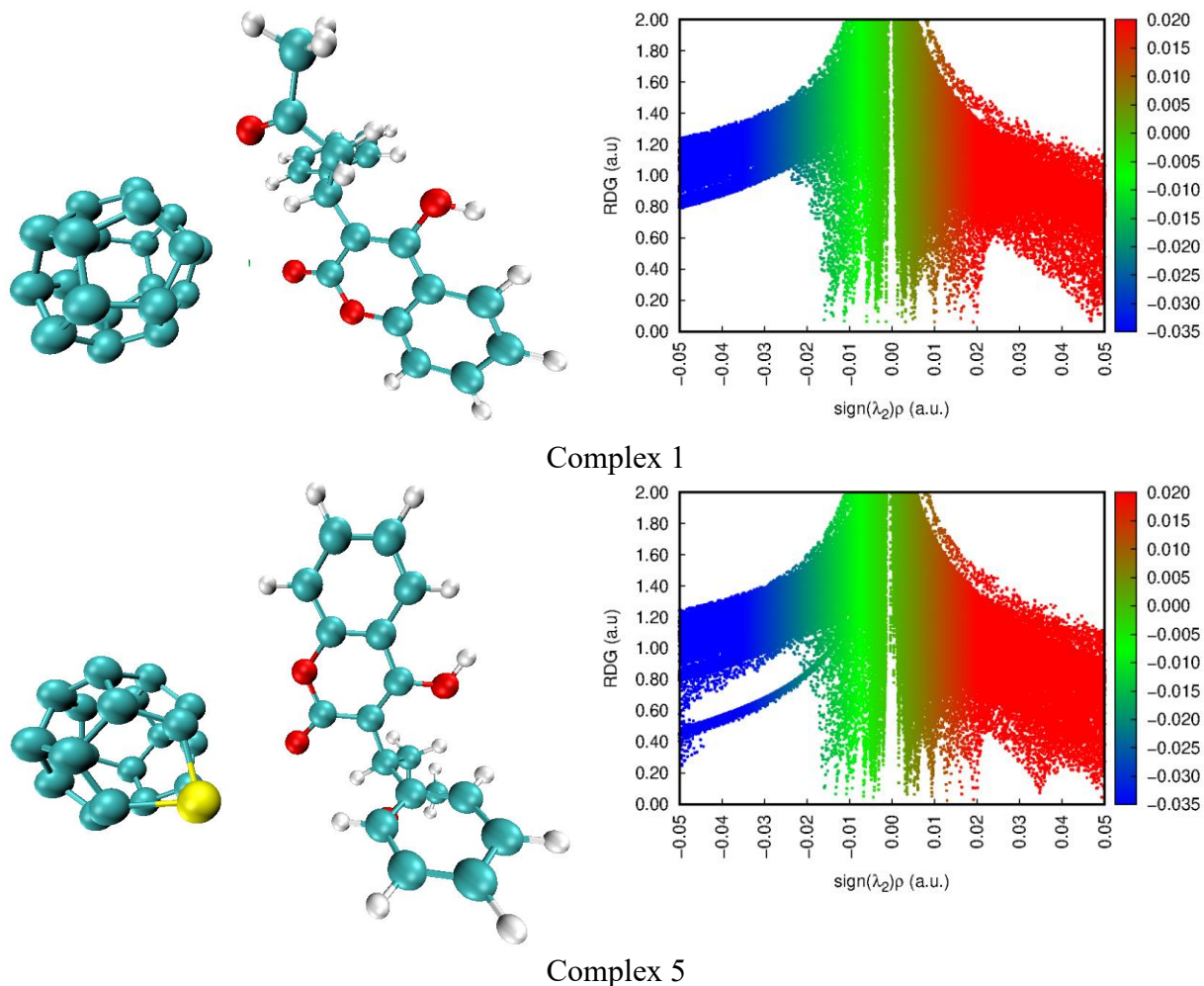


Fig. S4. The molecular graphs, RDG scatter maps, and color-filled IGMH δg^{inter} isosurface map of Complex 1 and Complex 5.