Development of Rational Synthetic Methodologies for Metallocarbohedrynes (Met-cars)

Our proposal was to develop rational syntheses of metallocarbohedrynes (met-cars) such as Ti_8C_{12} (pictured: carbon atoms are cyan, inner Ti atoms are grey, outer Ti atoms are brown), which had previously been known only in the gas phase at high temperatures.



Syntheses in the condensed phase are clearly desirable because examples of this class of compounds have or are expected to have ionization potentials between those of sodium and potassium, HOMO-LUMO gaps near zero! Thus the compounds in the condensed phase should be dark colored and may well exhibit metallic properties and extremely interesting chemistry. While we have not (yet) achieved unambiguous success in our synthetic endeavors, intensely colored materials which exhibit metallic luster have been obtained via various routes.