Properties of Negatively Charged Ruthenium Clusters in Molten Sodium Chloride

Negatively charged ruthenium clusters dispersed in molten NaCl are studied with density functional theory and molecular dynamics. The Ru clusters are charged by adding additional Na atoms to the molten salt. We consider Ru$_6^{m-}$ and 2Ru$_3$ clusters ($m = 0, 2, 4$) and investigate the importance of size, charge, and molten NaCl electrolyte on the stability of the small Ru clusters. Generally, the Ru clusters are not stable in the few atom limit compared to Ru atoms in bulk metallic Ru. However, charging the clusters, increasing their size, and solvating them in molten NaCl reduces the energy cost substantially. Neutral Ru$_6$ suspended in NaCl is relatively unreactive toward N$_2$ adsorption, but when charged, the clusters are predicted to be very active for both molecular and dissociative N$_2$ adsorption.