Ionisation Potentials of Metal Carbide Clusters

VIKTORAS DRYZA, Department of Chemistry, The University of Adelaide, South Australia 5005, Australia, M. ADDICOAT, JASON GASCOOKE, MARK BUNTINE, GREGORY METHA — Photo-Ionisation Efficiency (PIE) experiments have been performed on gas phase niobium and tantalum carbide clusters to determine their ionisation potentials (IPs). For TanCm (n = 3-4, m = 0-4) clusters an oscillatory behaviour is observed such that clusters with an odd number of carbon atoms have higher IPs and clusters with an even number of carbons have lower IPs. Excellent agreement is found with relative IPs calculated using density functional theory for the lowest energy structures, which are consistent with the development of a 2x2x2 face-centred nanocrystal. For the niobium carbide clusters we observe the species Nb4C5 and Nb4C6. Initial calculations suggest that these clusters contain carbon-carbon bonding. Interestingly, the stoichiometry for Nb4C6 is half that of a metcar, M8C12. Preliminary data will also be shown on bimetallic-carbide clusters.

Viktoras Dryza
Department of Chemistry, The University of Adelaide, South Australia 5005, Australia

Date submitted: 18 Jan 2006
Electronic form version 1.4