

Abstract Submitted  
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**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  $Ta_nC_m$  ( $n = 3-4$ ,  $m = 0-4$ ) 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  $2 \times 2 \times 2$  face-centred nanocrystal. For the niobium carbide clusters we observe the species  $Nb_4C_5$  and  $Nb_4C_6$ . Initial calculations suggest that these clusters contain carbon-carbon bonding. Interestingly, the stoichiometry for  $Nb_4C_6$  is half that of a metcar,  $M_8C_{12}$ . Preliminary data will also be shown on bimetallic-carbide clusters.

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