

# Structures of free transition metal cluster ions: Trapped ion electron diffraction and DFT calculations

*Detlef Schooß*

Institut für Nanotechnologie, Forschungszentrum Karlsruhe, D-76021 Karlsruhe, Germany

The structures of transition metal cluster ions have been studied by the recently developed technique of trapped ion electron diffraction (TIED)<sup>1</sup>. In brief, cluster ions are generated by a magnetron sputter source and injected into a cooled (95 K) quadrupole ion trap. After mass selection and thermalization, the trapped ions are irradiated with a 40 keV electron beam. The resulting diffraction pattern is integrated with a CCD detector. The assignment of the structural motif is done via a comparison of the experimental and simulated scattering function, calculated from density functional theory structure calculations.

The structures of mass selected silver cluster cations  $\text{Ag}_{19}^+$ ,  $\text{Ag}_{38}^+$ ,  $\text{Ag}_{55}^+$ ,  $\text{Ag}_{59}^+$ ,  $\text{Ag}_{75}^+$  and  $\text{Ag}_{79}^+$  have been investigated<sup>2</sup>. The resulting experimental data are best described by structures based on the icosahedral motif, while closed packed structures could be ruled out. Additionally, we present a comparison of the structures of  $\text{Cu}_{20}^{+/-}$ ,  $\text{Ag}_{20}^{+/-}$  and  $\text{Au}_{20}^{+/-}$ . Our findings show unambiguously that the structure of  $\text{Au}_{20}^-$  is predominantly given by a tetrahedron in agreement with previous results<sup>3</sup>. In contrast, structures of  $\text{Ag}_{20}^-$  and  $\text{Cu}_{20}^-$  based on the icosahedral motif agree best with the experimental data. Small structural differences between the charge states are observed. The possibilities and limitations of the TIED method are discussed.

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