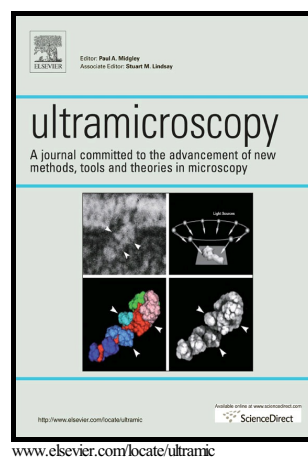


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ACCEPTED MANUSCRIPT

Exploring the Atomic Structure of 1.8 nm Monolayer-Protected Gold Clusters with Aberration-Corrected STEM

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Abstract

Monolayer-protected (MP) Au clusters present attractive quantum systems with a range of potential applications e.g. in catalysis. Knowledge of the atomic structure is needed to obtain a full understanding of their intriguing physical and chemical properties. Here we employed aberration-corrected scanning transmission electron microscopy (ac-STEM), combined with multislice simulations, to make a round-robin investigation of the atomic structure of chemically synthesized clusters with nominal composition $\text{Au}_{144}(\text{SCH}_2\text{CH}_2\text{Ph})_{60}$ provided by two different research groups. The MP Au clusters were “weighed” by the atom counting method, based on their integrated intensities in the high angle annular dark field (HAADF) regime and calibrated exponent of the Z dependence. For atomic structure analysis, we compared experimental images of hundreds of clusters, with atomic resolution, against a variety of structural models. Across the size range 123 to 151 atoms, only 3 percent of clusters matched the theoretically predicted

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