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First-Principles Investigation of Isolated Ultra-Thin Noble-Metal Polyhedral Nanowires SEAN MULLINS, XOCHITL LOPEZ-LOZANO, University of Texas, San Antonio — The theoretical investigation of high-stability structures at nanoscale is fundamental for the continuing development of novel nanomaterials. Ultra-thin nanowires are of great interest for they often have excellent mechanical, electrical, thermal, and optical properties, making them suitable for applications in nanodevices and nanomaterials for sensing, imaging, and cancer therapy. In this work we have performed Density Functional Theory (DFT) calculations to investigate the properties of gold and silver isolated nanowires using the SIESTA code. Our calculations show that nanowires configured with tetrahelical morphology exhibit metastability. When the tetrahelixes deform, a nanowire was obtained with octahedral components. Using these octahedrons as building blocks new polyhedral nanowires were constructed and optimized. A detailed description of their structural and electronic properties is presented.

Sean Mullins
University of Texas, San Antonio

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