

Abstract Submitted
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***I*-Au₆₀: Chiral Symmetry Breaking Yields a Perfect Golden Shell of Singular Rigidity** SEAN MULLINS, University of Texas, San Antonio, HANS-CHRISTIAN WEISSKER, Aix-Marseille Universit, J. JESUS PELAYO, Universidad Autnoma del Estado de Hidalgo, IGNACIO GARZON, Universidad Nacional Autnoma de Mxico, ROBERT WHETTEN, XOCHITL LOPEZ-LOZANO, University of Texas, San Antonio — The unique properties of elemental gold ($Z=79$, Au) derive from the extreme relativistic contraction of its atomic core $[Xe] 5d^{10}$ orbitals. Among these manifest properties are a propensity toward planarity, 2D bonding ($5d_{z^2} - 6s$ hybridization) and high electro-negativity (2.54) exceeding that of any other metallic or semi-metallic element. We report an astounding consequence: a chiral symmetry-breaking, i.e. the predicted spontaneous formation of a chiral-icosahedral shell (*I*-Au₆₀) from achiral (I_h) precursor forms, accompanied by a contraction in the Au-Au bonding and hence the radius of this *perfect golden sphere*, in which all 60 atomic sites are chemically equivalent. This structure, which resembles that most complex of semi-regular (Archimedean) polyhedra (3.3.3.5*), may be viewed as an optimal topological solution to the problem: how to close a 60-vertex 2D (triangular) net in 3D. The singular rigidity of the *I*-Au₆₀ manifests in uniquely discrete structural, vibrational, electronic, and optical signatures, which are reported as a guide to its experimental detection and ultimately its isolation in material forms. Its high (implicated) electronegativity suggests routes to obtaining it as a spherically aromatic *I*-Au₆₀^(6-,12-) salts of various inert counter-cations. Its large internal void could also hold a complex as large as I_h -M₁₂C₆₀, M = a mono- or di-valent metal ion.

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