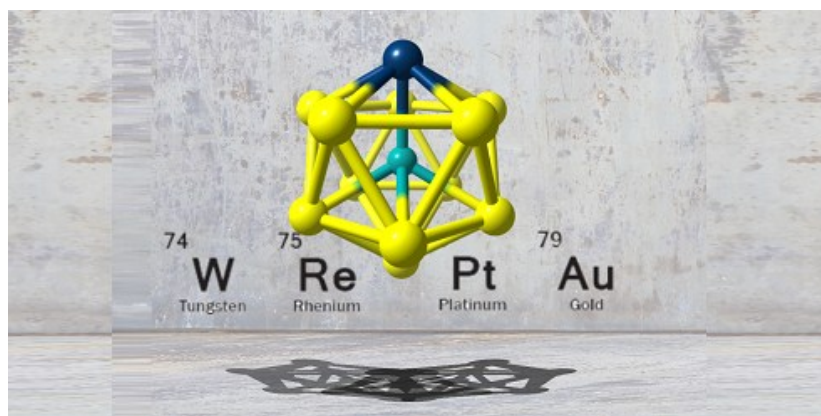


Doping the Cage. $\text{Re}@Au_{11}\text{Pt}$ and $\text{Ta}@Au_{11}\text{Hg}$, As Novel 18-*ve* Trimetallic Superatoms Displaying a Doped Icosahedral Golden Cage

Alvaro Muñoz-Castro



Content

Table S2. Coordinates (Å) of the optimized structures for $\text{Re}@Au_{11}\text{Pt}$ and $\text{Ta}@Au_{11}\text{Hg}$.

Table S1. Atomic orbital analysis of the superatomic shells.

Shell	W@Au ₁₂		Re@Au ₁₁ Pt		Ta@Au ₁₁ Hg	
1d	5d-Au	32.0%	5d-Au	21.0%	5d-Au	19.3%
	6s-Au	40.6%	6s-Au	28.9%	6s-Au	27.3%
			5d-Pt	21.0%	5d-Hg	13.4%
			6s-Pt	9.0%	6s-Hg	11.5%
	5d-W	27.4%	5d-Re	20.1%	5d-Ta	28.5%
1p	5d-Au	32.1%	5d-Au	32.0%	5d-Au	20.2%
	6s-Au	54.2%	6s-Au	37.8%	6s-Au	44.8%
			5d-Pt	0.0%	5d-Hg	8.3%
			6s-Pt	17.6%	6s-Hg	7.4%
	6p-W	13.7%	6p-Re	12.6%	6p-Ta	19.3%
1s	5d-Au	3.2%	5d-Au	1.6%	5d-Au	1.3%
	6s-Au	62.4%	6s-Au	59.0%	6s-Au	53.5%
			5d-Pt	1.3%	5d-Hg	16.9%
			6s-Pt	5.7%	6s-Hg	6.4%
	6s-W	34.3%	6s-Re	32.4%	6s-Ta	32.0%

Table S2. Coordinates (Å) of the optimized structures for Re@Au₁₁Pt and Ta@Au₁₁Hg.

13
Re@Au₁₁Pt

Au	-0.751046000	-2.311482000	-1.207268000
Au	-1.996634000	1.450640000	1.261579000
Au	1.966264000	-1.428574000	-1.207268000
Au	0.762646000	2.347184000	1.261579000
Au	-1.996634000	-1.450640000	1.261579000
Au	2.467976000	0.000000000	1.261579000
Au	-2.430436000	0.000000000	-1.207268000
Au	1.966264000	1.428574000	-1.207268000
Au	0.762646000	-2.347184000	1.261579000
Au	0.000000000	0.000000000	-2.783428000
Au	-0.751046000	2.311482000	-1.207268000
Pt	0.000000000	0.000000000	2.531958000
Re	0.000000000	0.000000000	0.007221000

13
Ta@Au₁₁Hg

Au	-1.993632000	-1.271592000	1.459946000
Au	-0.762169000	1.201487000	-2.360171000
Au	0.760535000	-1.260965000	2.347805000
Au	1.999337000	1.210030000	-1.463106000
Au	-2.478875000	1.203132000	0.011220000
Au	2.005693000	1.203762000	1.455348000
Au	-1.995261000	-1.265606000	-1.450182000

Au	2.467413000	-1.262814000	-0.012916000
Au	-0.766682000	1.214010000	2.355153000
Au	0.000910000	-2.737101000	0.003779000
Hg	-0.003218000	3.021001000	-0.001739000
Au	0.765910000	-1.273840000	-2.345333000
Ta	-0.002326000	0.018496000	0.000196000