

$R_{14}(\text{Au}, M)_{51}$ ($R = \text{Y, La-Nd, Sm-Tb, Ho, Er, Yb, Lu}$; $M = \text{Al, Ga, Ge, In, Sn, Sb, Bi}$): Stability Ranges and Site Preference in the $\text{Gd}_{14}\text{Ag}_{51}$ Structure Type

Chris Celandia,^{†,‡} Volodymyr Smetana,^{†,||} Alessia Provino,^{†,§,⊥} Pietro Manfrinetti,^{†,§,⊥} Anja-Verena Mudring^{†,‡,||*}

[†]*The Ames Laboratory, U.S. Department of Energy, Iowa State University, Ames, IA 50011, USA*

[‡]*Department of Materials Science and Engineering, Iowa State University, Ames, IA 50011, USA*

^{||}*Department of Materials and Environmental Chemistry, Stockholm University, Svante Arrhenius väg 16 C, 106 91 Stockholm, Sweden*

[§]*Department of Chemistry, University of Genova, Via Dodecaneso 31, 16146 Genova, Italy*

[⊥]*Institute SPIN-CNR, Corso Perrone 24, 16152 Genova, Italy*

Supporting information

Table S1. EDX analyses of the Gd₁₄Ag₅₁-type compounds in the R-Au-M systems. Atomic percentages are within 1 at.% accuracy and support projected elemental compositions based on single crystal refinement.

Sample	<i>R</i> [at.%]	Au [at.%]	<i>M</i> [at.%]
La-Au-Bi	21.34	76.44	2.22
Nd-Au-Ga	21.72	69.48	8.81
Sm-Au-Bi	20.96	76.91	2.13
Gd-Au-Sn	22.03	70.81	7.17
Ho-Au-Ge	21.39	69.82	8.78
Ho-Au-Sb	22.48	68.48	9.04
Lu-Au-Ga	21.37	54.13	24.5

Table S1. Lattice parameters data as obtained by powder X-ray diffraction.

Sample	Lattice parameters		<i>V</i> _{obs} [Å ³]
	<i>a</i> [Å]	<i>c</i> [Å]	
Nd ₁₄ Au _{45.6} Ga _{5.4}	12.6888(2)	9.2184(3)	1285.37(4)
Gd ₁₄ Au _{46.9} Sn _{4.1}	12.6958(1)	9.1960(1)	1283.7(1)
Ho ₁₄ Au _{45.3} Ge _{5.7}	12.4888(2)	9.0812(3)	1226.64(4)
Ho ₁₄ Au _{45.1} Sb _{5.9}	12.6192(1)	9.1869(1)	1267.0(1)
Lu ₁₄ Au _{35.3} Ga _{15.7}	12.3136(2)	8.9967(3)	1181.35(4)

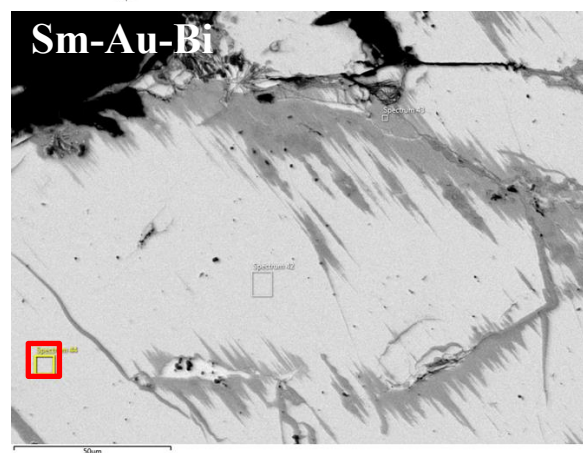
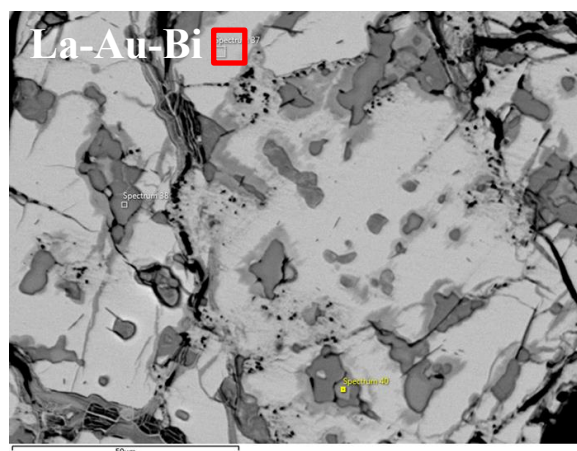
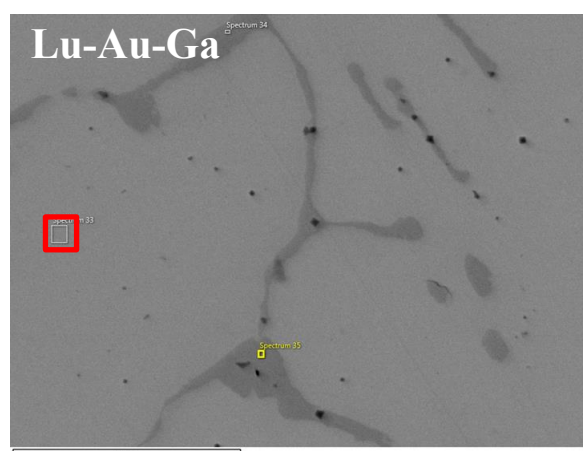
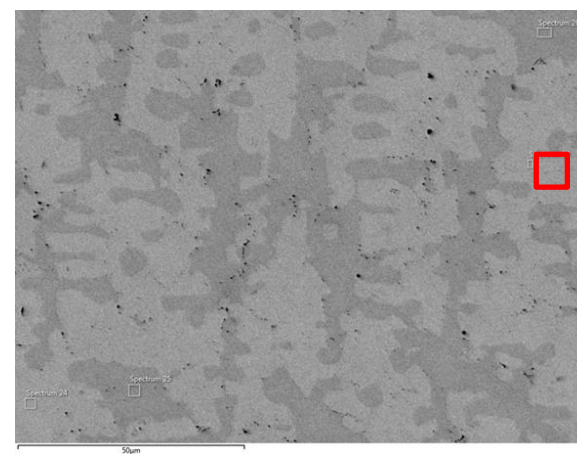
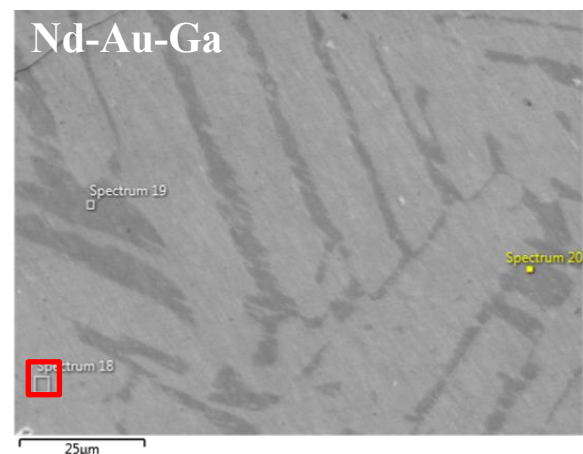
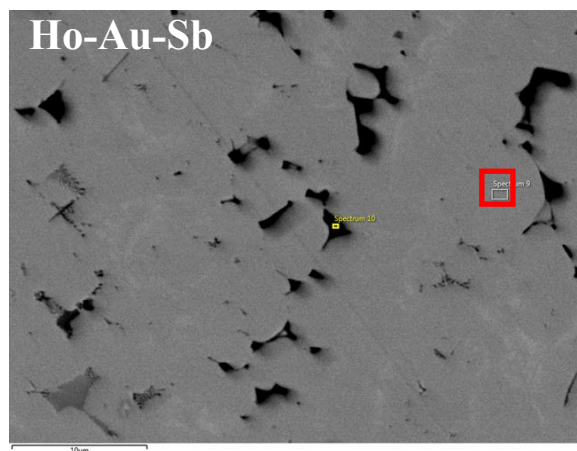
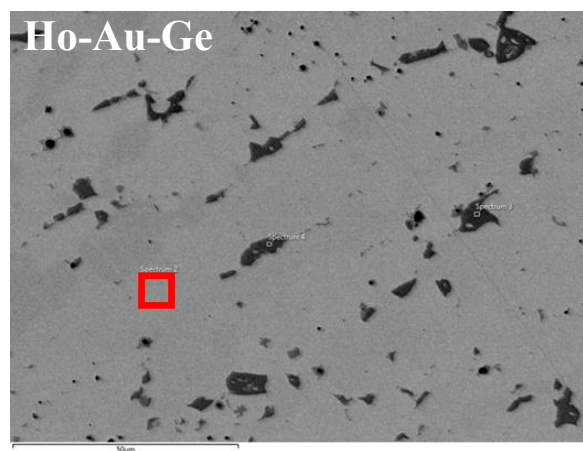


Figure S1. SEM micrographs (backscattered electron mode, BSE) of various samples used for EDS analysis. Regions used for EDS data from Table S1 are highlighted in red for each sample. Generally, the light grey grains are the $Gd_{14}Ag_{51}$ -type compound, while the darker phase is pertaining to the $R(Au_{1-x}M_x)_3$ phase.

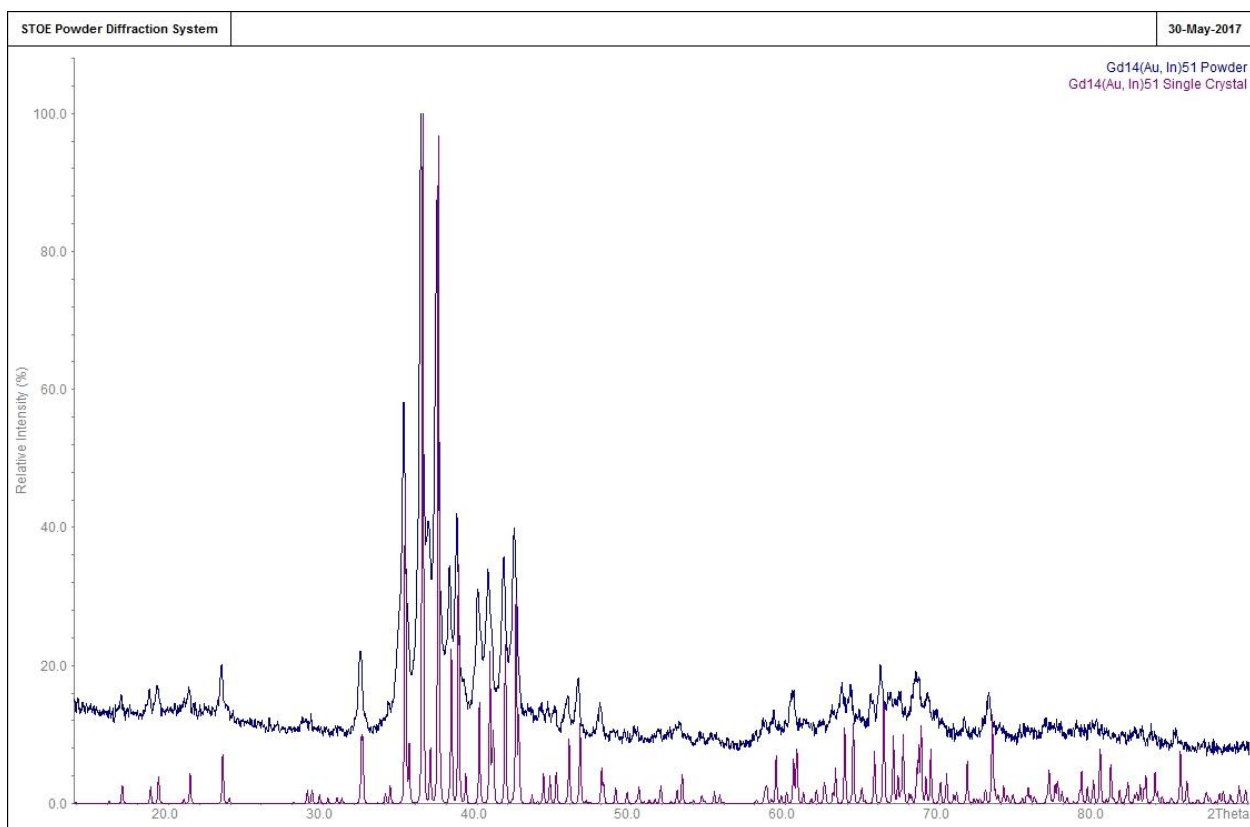


Figure S2. Comparison of powder X-ray diffraction data and theoretical peaks from corresponding single crystal X-ray diffraction data from Gd-Au-In sample.

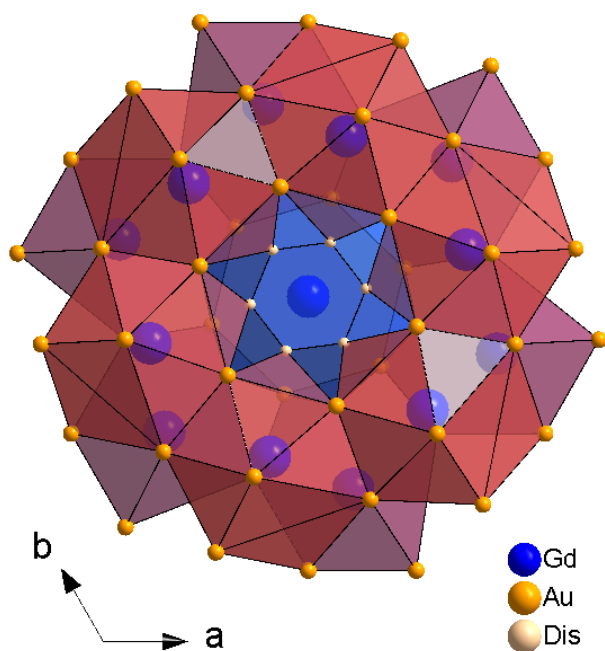


Figure S3. Alternate perspective of rare earth coordination polyhedra stacking scheme showing polyhedral “wheels” of the slab layers surrounding the columns of face-sharing double $R2$ coordination polyhedra.

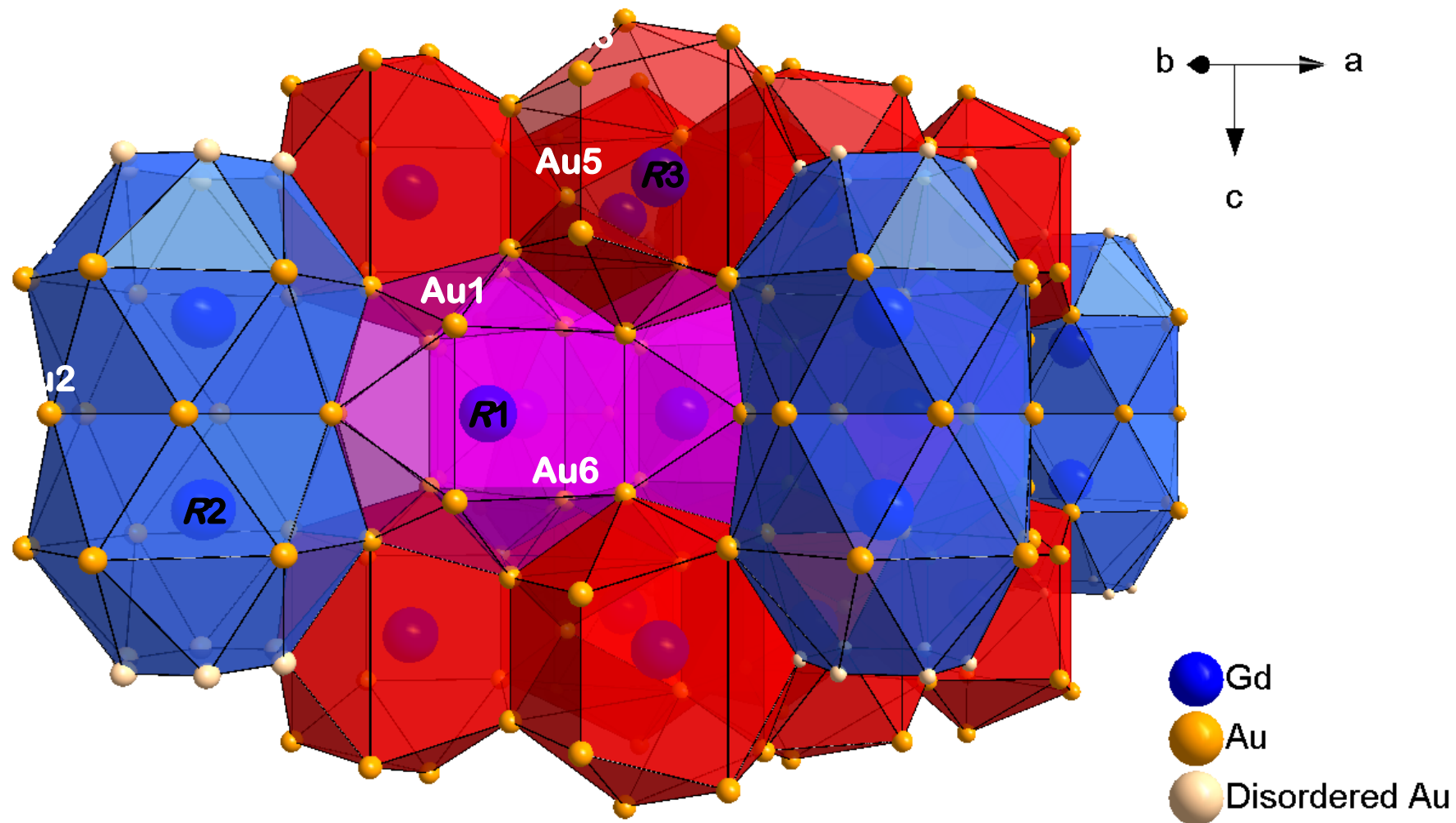


Figure S4. $\text{Gd}_{14}\text{Au}_{51}$ structure with atomic sites labeled for clarity. $R1$ and $R3$ polyhedra have been made more translucent in order to resolve atomic sites that are located toward the center of the unit cell.

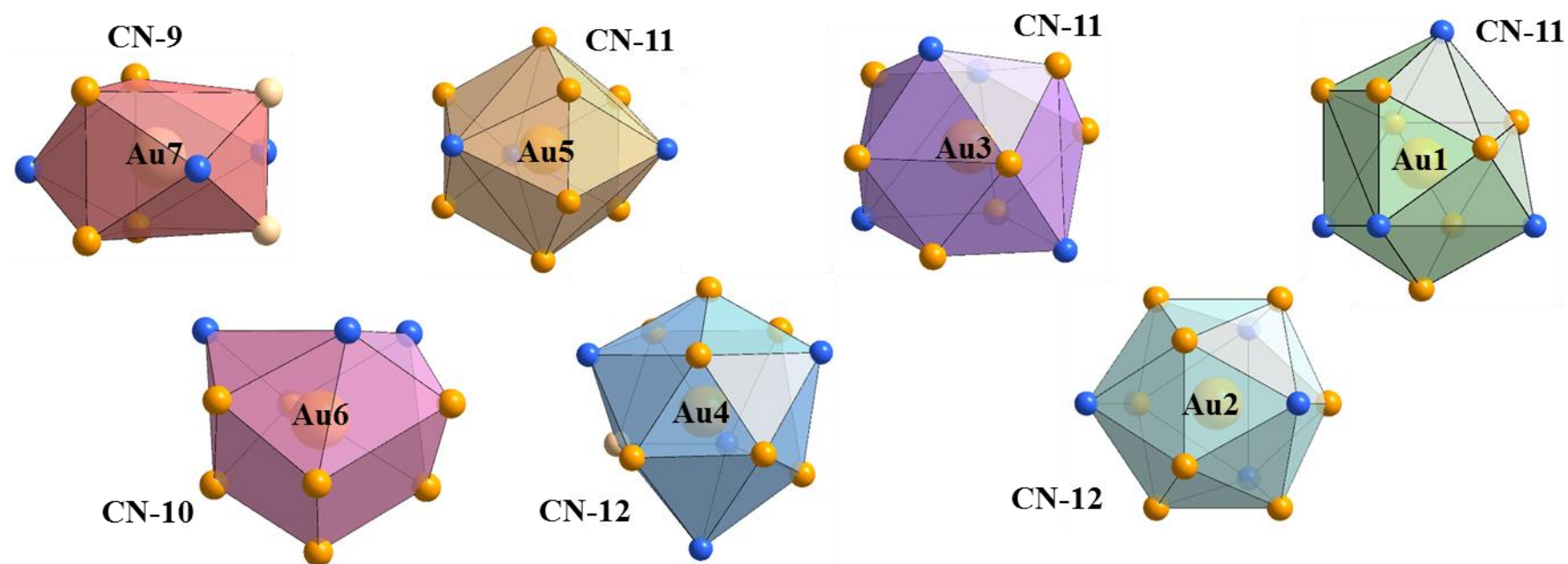


Figure S5. Au coordination polyhedra and coordination numbers.