

***Structural and morphological peculiarities of hybrid Au/nanodiamond  
engineered nanostructures***

***SUPPORTING INFORMATION***

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## Supporting Information.

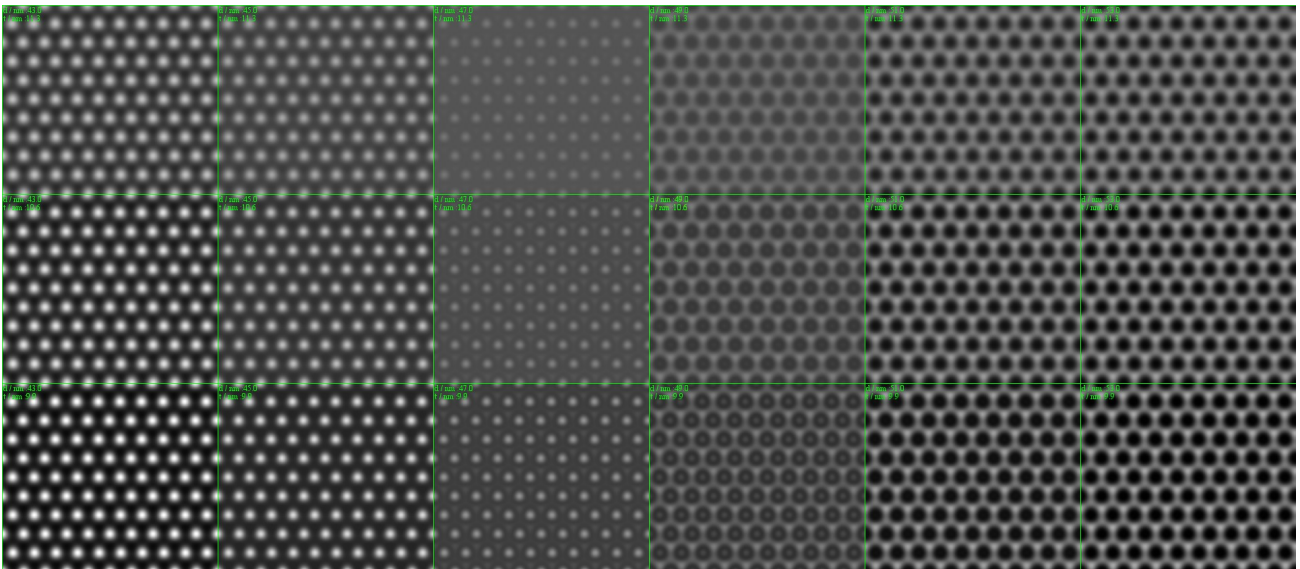
**Table S1.** Interplanar spacing (nm) of observed reflections for Au-ND nanocomposite of figure 2b and 3d with  $d_{111}$  of NDIA as standard calibration. Miller indexes and corresponding reference data of Au (card PDF#00-002-1095), ND (card PDF#0675 and reference [A]), and Graphite (card PDF 41-1487).

$N_{\text{Rings}}$	Measured	hkl	Gold	Diamond	hkl	Graphite
1	0.2362	111	0.236	—	002	3.354
2	0.2061	111	—	0.206	100	2.131
3	0.2044	200	0.204	—	101	2.031
4	0.1740	200	—	—	102	1.798
5	0.1450	220	0.144	—	004	1.677
6	0.1261	220	—	0.126	103	1.542
7	0.1231	311	0.123	—	110	1.230
8	0.1174	222	0.117	—	112	1.155
9	0.1086	311	—	0.108	105	1.135
10	0.1036	222	0.102	—	006	1.118
11	0.0932	331	0.093	—		
12	0.0916	420	0.091	—		
13	0.0893	400	—	0.089		
14	0.0834	422	0.083	—		
15	0.0823	313	—	0.082		
16	0.0802	204	—	—		
17	0.0784	511	0.078	—		
18	0.7350	224	—	0.073		

## High resolution transmission electron microscopy simulations

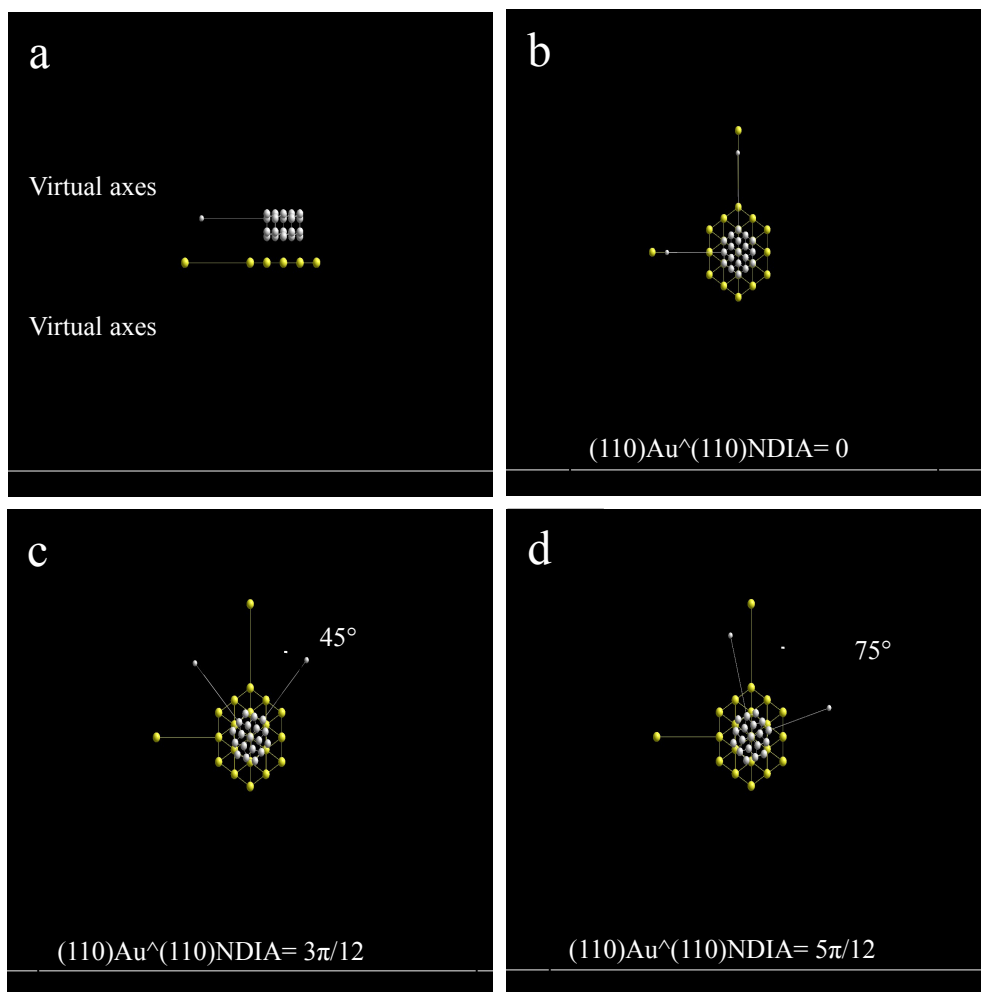
The multislice method was employed to simulate HREM image of gold nanoparticle. The simulations conditions were referred to the HR-TEM instrument (JEOL JEM-3000F FEG TEM): acceleration voltage 300 kV, spherical aberration of  $C_s=0.6$  mm, three-fold astigmatism of 850 nm, beam divergence of 0.10 mrad and focal spread of 5 nm.

Multislice simulations were conducted for a 15 nm thick gold crystal in [111] zone axis of a supercell of 5x5 unit cells. Defocus series were calculated with an objective aperture of 12.2 mrad setting 2.0 nm defocus step, being the starting defocus around -41.0 nm according to the Scherzer focus parameter of the TEM.



**Figure 1S.** HREM defocus-thickness map image of gold atomic layer.

[A] M. L. Terranova, D. Manno, M. Rossi, A. Serra, E. Filippo, S. Orlanducci, and E. Tamburri, *Cry. Growth Des.*, **2009**, *9*, 1245-1249.



**Figure 2S.** Atomic sketch views of two NDIA layers (white balls) stacked on one gold layer (yellow balls) both oriented along the [111] zone axis. a) Au and NDIA layers separated by non-covalent bonding (Van der Waals interactions). b)  $(110)Au^{(110)NDIA} = 0$  radian. c)  $(110)Au^{(110)NDIA} = 3\pi/12$  radians. d)  $(110)Au^{(110)NDIA} = 5\pi/12$  radians.